

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: LEE, RIL A. Examiner #: 78680 Date: JULY 6, 2004
Art Unit: 4743 Phone Number: 571-272-1104 Serial Number: 10/624,679
Mail Box and Bldg/Room Location: REM10A24 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: ACENAPHTHYLENE DERIVATIVE, POLYMER, and ANTI-REFLECTIVE COMPOSITION

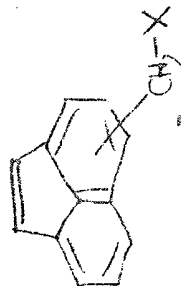
Inventors (please provide full names): SUGITA, H. KONNO, K.

TANAKA, M. SHIMOKAWA, T.

Earliest Priority Filing Date: July 31, 2002

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

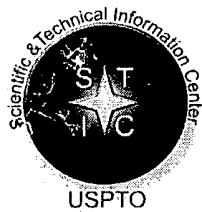
Please search for acenaphthylene derivatives having the following general formula



must have methylene group

X can be anything

substituent CH₂X located on either six membered ring



STIC Search Report

EIC 1700

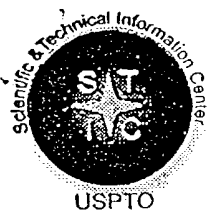
STIC Database Tracking Number: 126545

**TO: Rip A Lee
Location: REM 10A24
Art Unit : 1713
July 12, 2004**

Case Serial Number: 10/624670

**From: Kathleen Fuller
Location: EIC 1700
REMSSEN 4B28
Phone: 571/272-2505
Kathleen.Fuller@uspto.gov**

Search Notes



STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact *the EIC searcher or contact:*

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

- I am an examiner in Workgroup: Example: 1713
➤ Relevant prior art **found**, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
(journal articles, conference proceedings, new product announcements etc.)

- Relevant prior art **not found**:

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to EIC1700 REMSEN 4B28



SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: LEE, RLP A. Examiner #: 78680 Date: JULY 6, 2004
 Art Unit: 1713 Phone Number: 571-272-1104 Serial Number: 10/624,673
 Mail Box and Bldg/Room Location: REM10A24 Results Format Preferred (circle): PAPER DISK E-MAIL

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

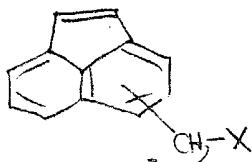
Title of Invention: ACENAPHTHYLENE DERIVATIVE, POLYMER, and ANTI-REFLECTIVE COMPOSITION

Inventors (please provide full names): SUGITA, H. KONNO, K.
TANAKA, M. SHIMOKAWA, T.

Earliest Priority Filing Date: July 31, 2002

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for acenaphthylene derivatives having the following general formula



Must have methylene group
 X can be anything

Substituent CH₂X located on either six membered ring

STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: _____	NA Sequence (#) _____	STN _____
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) _____	Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic _____	Dr.Link _____
Date Completed: _____	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>20</u>	Fulltext _____	Sequence Systems _____
Clerical Prep Time: _____	Patent Family _____	WWW/Internet _____
Online Time: <u>20</u>	Other _____	Other (specify) _____

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STRUCTURE FILE UPDATES: 11 JUL 2004 HIGHEST RN 708207-86-7
DICTIONARY FILE UPDATES: 11 JUL 2004 HIGHEST RN 708207-86-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> FILE HCAPLUS

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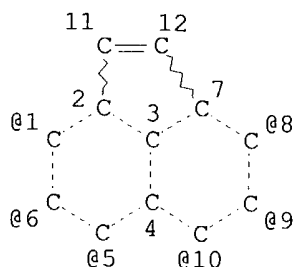
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FILE COVERS 1907 - 12 Jul 2004 VOL 141 ISS 3
FILE LAST UPDATED: 11 Jul 2004 (20040711/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> D QUE L53

L50 STR



*76 structures from
this query*

CH2 @13

VPA 13-8/9/10/5/6/1 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L52 76 SEA FILE=REGISTRY SSS FUL L50
L53 39 SEA FILE=HCAPLUS ABB=ON L52

39 CA references

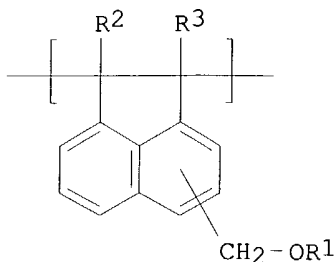
=> D L53 BIB ABS HITIND HITSTR 1-39

L53 ANSWER 1 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:97225 HCAPLUS
DN 140:136438
TI Acenaphthylene derivative, polymer, and antireflection film-forming
composition
IN Sugita, Hikaru; Konno, Keiji; Tanaka, Masato; Shimokawa, Tsutomu
PA JSR Corporation, Japan
SO Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW

DT Patent
LA English
FAN.CNT 1

applicant

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1386904	A1	20040204	EP 2003-17282	20030730
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	US 2004034155	A1	20040219	US 2003-624678	20030723
	JP 2004168748	A2	20040617	JP 2003-283561	20030731
PRAI	JP 2002-224138	A	20020731		
	JP 2002-324709	A	20021108		
OS	MARPAT 140:136438				
GI					



AB Novel compds. acetoxymethylacenaphthylene and hydroxymethylacenaphthylene are disclosed. A polymer prepared from these novel compds. contains a structural unit of the formula I (R1 = H; R2,3 = monovalent atom or a monovalent organic group). The polymer is suitable as a component for an antireflection film-forming composition exhibiting a high antireflection effect and not causing intermixing with a resist film.

IC ICM C07C033-38
ICS C08F232-08; G03F007-09

CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 76

IT 510754-50-4P 650624-82-1P **650624-84-3P** 650624-86-5P
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(acenaphthylene derivative and polymer for antireflection film-forming composition)

IT **650624-84-3P**
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(acenaphthylene derivative and polymer for antireflection film-forming composition)

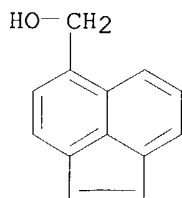
RN 650624-84-3 HCAPLUS

CN 5-Acenaphthylenemethanol, polymer with acenaphthylene (9CI) (CA INDEX NAME)

CM 1

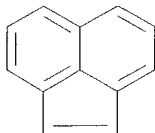
CRN 650624-83-2

CMF C13 H10 O



CM 2

CRN 208-96-8
CMF C12 H8



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 2 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:834012 HCAPLUS
DN 138:60408
TI Investigation of the Volatile Organic Substances that Cause the
Characteristic Odor of Pentachlorophenol Treated Wood Utility Poles
AU Fortin, Myriam; Gilbert, Roland; Besner, Andre; Labrecque, Jean-Francois;
Hubert, Joseph
CS Institut de Recherche d'Hydro-Quebec, Varennes, QC, J3X 1S1, Can.
SO Environmental Science and Technology (2002), 36(23), 5014-5020
CODEN: ESTHAG; ISSN: 0013-936X
PB American Chemical Society
DT Journal
LA English
AB The nature of volatile organic compds. which could be the origin of the
characteristic odor of treated wood utility poles was studied by examining
compositional changes in the chromatog. profiles of fresh
pentachlorophenol (PCP) solvent samples and weathered samples collected
from an in-service red pine pole. More than 99 peaks were identified in
the fresh solvent chromatogram from which a large portion of the C3-, C4-,
C5-, C6-alkylbenzene isomers and early eluting n-alkanes was missing from
the anal. of weathered samples. Three domains in the chromatog. profile
(volatile, semi-volatile, non-volatile components) were confirmed by
assessing the headspace of fresh PCP solvent samples using direct syringe
sampling and solid-phase micro-extraction. A first level of field validation
was achieved using an emission cell to measure substances emanating from
sapwood specimens at different temps. Average latent heat of vaporization
(ΔH_{vap}) of PCP solvent components was estimated to be 99.9 kJ/mol from
these results. Anal. of airborne substances at a treating plant and
utility pole storage site confirmed the C4-, C5-, and C6-alkylbenzene
isomers could contribute to the characteristic odor perceived by humans.
CC 59-2 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 43, 80
IT 71-43-2, Benzene, analysis 83-32-9, Acenaphthene 85-01-8,
Phenanthrene, analysis 86-73-7, Fluorene 90-12-0, 1-Methylnaphthalene
91-20-3, Naphthalene, analysis 91-57-6, 2-Methylnaphthalene 92-52-4,
Biphenyl, analysis 95-47-6, o-Xylene, analysis 95-63-6,
1,2,4-Trimethylbenzene 95-93-2, 1,2,4,5-Tetramethylbenzene 98-82-8,
Isopropylbenzene 99-87-6, p-Cymene 100-41-4, Ethylbenzene, analysis
103-65-1, Propylbenzene 104-51-8, 1-Butylbenzene 105-05-5,
1,4-Diethylbenzene 106-42-3, p-Xylene, analysis 108-38-3, m-Xylene,
analysis 108-67-8, 1,3,5-Trimethylbenzene, analysis 108-88-3, Toluene,
analysis 112-40-3, Dodecane 112-95-8, Eicosane 119-64-2,
1,2,3,4-Tetrahydronaphthalene 120-12-7, Anthracene, analysis 124-18-5,
Decane 135-01-3, 1,2-Diethylbenzene 135-98-8, sec-Butylbenzene

141-93-5, 1,3-Diethylbenzene 208-96-8, Acenaphthylene 275-51-4, Azulene 475-03-6, 1,2,3,4-Tetrahydro-1,1,6-trimethylnaphthalene 488-23-3, Benzene, 1,2,3,4-Tetramethyl- 490-65-3, Naphthalene, 1-Methyl-7-(1-methylethyl)- 496-11-7, 2,3-Dihydro-1H-indene 527-53-7, 1,2,3,5-Tetramethylbenzene 535-77-3, m-Cymene 538-68-1, Amylbenzene 544-76-3, Hexadecane 575-41-7, 1,3-Dimethylnaphthalene 581-40-8, 2,3-Dimethylnaphthalene 581-42-0, 2,6-Dimethylnaphthalene 593-45-3, Octadecane 611-14-3, 1-Ethyl-2-methylbenzene 613-33-2, 4,4'-Dimethylbiphenyl 620-14-4, 1-Ethyl-3-methylbenzene 629-50-5, Tridecane 629-59-4, Tetradecane 629-62-9, Pentadecane 629-78-7, Heptadecane 629-92-5, Nonadecane 629-94-7, Heneicosane 629-97-0, Docosane 629-99-2, Pentacosane 638-67-5, Tricosane 646-31-1, Tetracosane 767-58-8, 2,3-Dihydro-1-methyl-1H-indene 781-43-1, 9,10-Dimethylantracene 832-69-9, 1-Methylphenanthrene 874-41-9, 1-Ethyl-2,4-dimethylbenzene 934-74-7, 1-Ethyl-3,5-dimethylbenzene 934-80-5, 4-Ethyl-1,2-dimethylbenzene 939-27-5, 2-Ethyl-naphthalene 1074-17-5, 1-Methyl-2-propylbenzene 1074-43-7, 1-Methyl-3-propylbenzene 1074-55-1, 1-Methyl-4-propylbenzene 1075-22-5 1076-61-5, 1,2,3,4-Tetrahydro-6,7-dimethylnaphthalene 1077-16-3, Hexylbenzene 1120-21-4, Undecane 1127-76-0, 1-Ethyl-naphthalene 1207-15-4 1430-97-3, 2-Methyl-9H-fluorene 1559-81-5, 1,2,3,4-Tetrahydro-1-methylnaphthalene 1576-67-6, 3,6-Dimethylphenanthrene 1595-16-0, Benzene, 1-Methyl-4-(1-methylpropyl)- 1758-85-6, Benzene, 2,4-Diethyl-1-methyl- 1758-88-9, 2-Ethyl-1,4-dimethylbenzene 1921-70-6, 2,6,10,14-Tetramethylpentadecane 2027-17-0, Naphthalene, 2-(1-Methylethyl)- 2245-38-7, 2,3,5-Trimethylnaphthalene 2809-64-5, 1,2,3,4-Tetrahydro-5-methylnaphthalene 3031-15-0, 1,2,3,4-Tetramethylnaphthalene 3674-66-6, 2,5-Dimethylphenanthrene 3877-19-8, 1,2,3,4-Tetrahydro-2-methylnaphthalene 4175-54-6, Naphthalene, 1,2,3,4-Tetrahydro-1,4-dimethyl- 4612-63-9, 2,3-Dimethyl-9H-fluorene 6682-71-9 13065-07-1, Naphthalene, 1,2,3,4-Tetrahydro-2,7-dimethyl- 16587-52-3, 3-Methyldibenzothiophene 17059-48-2 21164-95-4, 7,9-Dimethylhexadecane 21564-91-0, 1,2,3,4-Tetrahydro-1,5-dimethylnaphthalene 21693-54-9, 1,2,3,4-Tetrahydro-5,7-dimethylnaphthalene 21693-55-0, Naphthalene, 1,2,3,4-Tetrahydro-1,5,7-trimethyl- 25550-13-4, Diethylmethylbenzene 28652-77-9, Trimethylnaphthalene 30316-17-7, 1,2,3,4-Tetrahydro-2,5,8-trimethylnaphthalene 33930-85-7 40650-41-7 42775-75-7, 5-Ethyl-1,2,3,4-tetrahydronaphthalene 56147-63-8 **132118-73-1**, Acenaphthylene, 1,2,5,6-Tetramethyl-

RL: ANT (Analyte); OCU (Occurrence, unclassified); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)

(volatile organic compds. causing characteristic odor from pentachlorophenol-treated wood utility poles determined by measuring compositional changes in chromatog. profiles of fresh and weathered solvent samples)

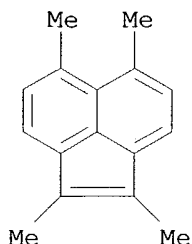
IT **132118-73-1**, Acenaphthylene, 1,2,5,6-Tetramethyl-

RL: ANT (Analyte); OCU (Occurrence, unclassified); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)

(volatile organic compds. causing characteristic odor from pentachlorophenol-treated wood utility poles determined by measuring compositional changes in chromatog. profiles of fresh and weathered solvent samples)

RN 132118-73-1 HCAPLUS

CN Acenaphthylene, 1,2,5,6-tetramethyl- (9CI) (CA INDEX NAME)



RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 3 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:547252 HCAPLUS

DN 137:109970

TI Acenaphthylene ring-containing crosslinkable compounds, their intermediates, their manufacture, and cured products

IN Honda, Hiroshi

PA Hitachi Chemical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002205967	A2	20020723	JP 2001-3423	20010111
PRAI	JP 2001-3423		20010111		

OS MARPAT 137:109970

AB Crosslinkable compds. (QCH₂O)_nR (I; Q = acenaphthylen-5-yl; n = pos. integer; R = n-valent organic group) and their intermediates QCH₂X (II; Q = same as I; X = halo) are claimed. Thus, etherification of 4,4'-dihydroxydiphenyl ether with II (X = Cl) gave 55.8% I (n = 2, R = p-C₆H₄OC₆H₄-p), which gave a cured product at 151°.

IC ICM C07C043-285

ICS C07C017-357; C07C022-04; C07C041-16; C08F032-08; C08K005-06; C08L101-00

CC 37-2 (Plastics Manufacture and Processing)

Section cross-reference(s): 25

IT **443282-80-2P**

RL: IMF (Industrial manufacture); PREP (Preparation)

(manufacture of acenaphthylene ring-containing crosslinkable compds. and their intermediates)

IT 5345-46-0P, 5-Formylacenaphthene 50773-22-3P 62456-13-7P,

5-Chloromethylacenaphthene **443282-78-8P 443282-79-9P**

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(manufacture of acenaphthylene ring-containing crosslinkable compds. and their intermediates)

IT **443282-80-2P**

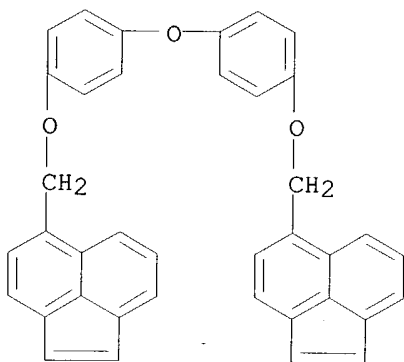
RL: IMF (Industrial manufacture); PREP (Preparation)

(manufacture of acenaphthylene ring-containing crosslinkable compds. and their intermediates)

RN 443282-80-2 HCAPLUS
CN Acenaphthylene, 5,5'-[oxybis(4,1-phenyleneoxymethylene)]bis-, homopolymer
(9CI) (CA INDEX NAME)

CM 1

CRN 443282-79-9
CMF C38 H26 O3



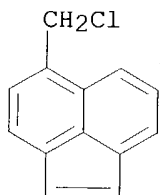
IT 443282-78-8P 443282-79-9P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
(Reactant or reagent)

(manufacture of acenaphthylene ring-containing crosslinkable compds. and
their intermediates)

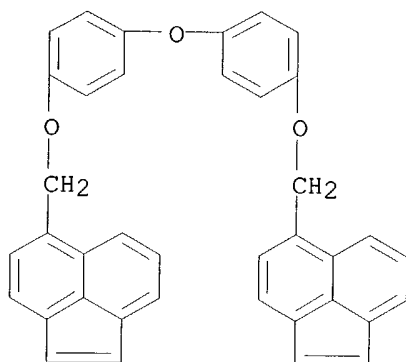
RN 443282-78-8 HCAPLUS

CN Acenaphthylene, 5-(chloromethyl)- (9CI) (CA INDEX NAME)

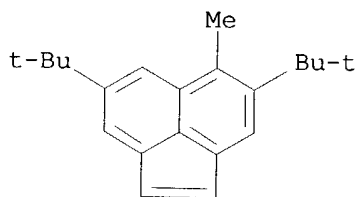


RN 443282-79-9 HCAPLUS

CN Acenaphthylene, 5,5'-[oxybis(4,1-phenyleneoxymethylene)]bis- (9CI) (CA
INDEX NAME)

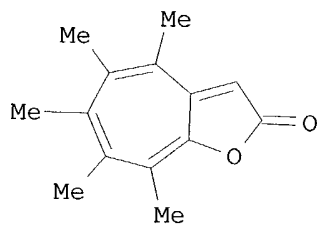


L53 ANSWER 4 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 2001:779945 HCAPLUS
 DN 136:232106
 TI Tetra-tert-butyl-as-indaceno[1,2,3-cd:6,7,8-c'd']diphenalene: a four-stage amphoteric redox system
 AU Kubo, Takashi; Yamamoto, Kagetoshi; Nakasuji, Kazuhiro; Takui, Takeji
 CS Graduate School of Science, Department of Chemistry, Osaka University, Toyonaka, 560-0043, Japan
 SO Tetrahedron Letters (2001), 42(45), 7997-8001
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 OS CASREACT 136:232106
 AB Tetra-tert-butyl-as-indaceno[1,2,3-cd:6,7,8-c'd']diphenalene (TTB-as-IDPL) was prepared and found to behave as a four-stage amphoteric redox compound. The properties of its five redox states were investigated. Properties of the newly synthesized compound were compared to the known, sym. 4,8,12,16-tetrakis(1,1-dimethylethyl)benz[5,6]acenaphtho[1,2-k]benzo[cd]fluoranthene.
 CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds) Section cross-reference(s): 22
 IT 105-53-3, Diethyl malonate 108-31-6, Maleic anhydride, reactions 203726-97-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of tetra-tert-butyl-as-indaceno[1,2,3-cd:6,7,8-c'd']diphenalene and its properties as four-stage amphoteric redox system)
 IT 203726-97-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of tetra-tert-butyl-as-indaceno[1,2,3-cd:6,7,8-c'd']diphenalene and its properties as four-stage amphoteric redox system)
 RN 203726-97-0 HCAPLUS
 CN Acenaphthylene, 4,7-bis(1,1-dimethylethyl)-5-methyl- (9CI) (CA INDEX NAME)



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 5 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:561252 HCAPLUS
DN 135:318178
TI Surprising formation of highly substituted azulenes on thermolysis of
4,5,6,7,8-pentamethyl-2H-cyclohepta[b]furan-2-one and heptalene formation
with the new azulenes
AU Lellek, Vit; Hansen, Hans-Jurgen
CS Organisch-chemisches Institut der Universitat Zurich, Zurich, CH-8057,
Switz.
SO Helvetica Chimica Acta (2001), 84(6), 1712-1736
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
OS CASREACT 135:318178
GI



AB Heating of 4,5,6,7,8-pentamethyl-2H-cyclohepta[b]furan-2-one (1a, I) in decalin at temps. > 170° leads to the development of a blue color, typical for azulenes. It belongs, indeed, to two formed azulenes, namely 4,5,6,7,8-pentamethyl-2-(2,3,4,5,6-pentamethylphenyl)azulene (4a) and 4,5,6,7,8-pentamethylazulene (5a). As a third product, 4,5,6,7-tetramethyl-2-(2,3,4,5,6-pentamethylphenyl)-1H-indene (6a) is also found in the reaction mixture. Neither 4,6,8-trimethyl-2H-cyclohepta[b]furan-2-one (1b) nor 2H-cyclohepta[b]furan-2-one (1c) exhibit, on heating, such reactivity. However, heating of mixts. 1a/1b or 1a/1c results in the formation of crossed azulenes, namely 4,6,8-trimethyl-2-(2,3,4,5,6-pentamethylphenyl)azulene (4ba), resp. and 2-(2,3,4,5,6-pentamethylphenyl)azulene (4ca), resp. The formation of small amts. of 4,6,8-trimethylazulene (5ba) and azulene (5ca), resp., besides 1H-indene 6a is also observed. The observed product types speak for an [8+2]-cycloaddn. reaction between two mols. of 1a or between 1b and 1c, resp., with 1a, whereby 1a plays in the latter two cases the part of the two-atom component. Strain release, due to the five adjacent Me groups in 1a, in the [8+2]-cycloaddn. step seems to be

the driving force for these transformations, which are further promoted by the consecutive loss of two mols. of CO₂ and concomitant formation of the 10 π -electron system of the azulenes. The new azulenes react with di-Me acetylenedicarboxylate (ADM) to form the corresponding di-Me heptalene-4,5-dicarboxylates, which give thermally or photochem. the corresponding double-bond-shifted (DBS) isomers. The five adjacent Me groups in exert a certain buttressing effect, whereby their thermal DBS process is distinctly retarded in comparison to rings which carry "isolated" Me groups. This view is supported by X-ray crystal-structure analyses.

CC 22-5 (Physical Organic Chemistry)

Section cross-reference(s): 75

IT **367452-56-0P**

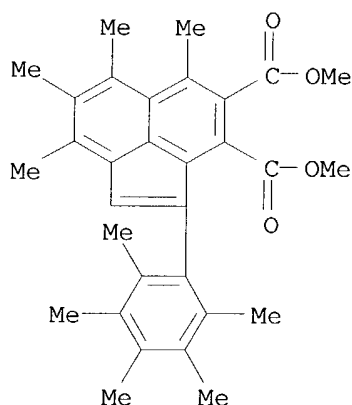
RL: BYP (Byproduct); PRP (Properties); PREP (Preparation) (crystallog.; preparation of azulenes via chemoselective [2+8]-cycloaddn./cycloreversion/ring contraction from 2H-cyclohepta[b]furan-2-ones, and heptalene bond-shift isomers from the new azulenes + DMAD)

IT **367452-56-0P**

RL: BYP (Byproduct); PRP (Properties); PREP (Preparation) (crystallog.; preparation of azulenes via chemoselective [2+8]-cycloaddn./cycloreversion/ring contraction from 2H-cyclohepta[b]furan-2-ones, and heptalene bond-shift isomers from the new azulenes + DMAD)

RN 367452-56-0 HCAPLUS

CN 3,4-Acenaphthylenedicarboxylic acid, 5,6,7,8-tetramethyl-2-(pentamethylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 6 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

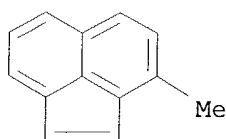
AN 1999:231997 HCAPLUS

DN 130:303552

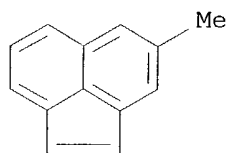
TI Classification of select aceanthrylenes, acephenanthrylenes, and dicyclopentapyrenes as alternant versus nonalternant polycyclic aromatic hydrocarbons on the basis of their fluorescence quenching behavior in the presence of nitromethane and cetylpyridinium cation selective quenching agents

AU Pandey, Siddharth; Acree, William E., Jr.; Scott, Lawrence T.; Necula, Atena; Fetzer, John C.; Mulder, Patrick P. J.; Lugtenburg, Johan;

Cornelisse, Jan
 CS Department Chemistry, University North Texas, Denton, TX, 76203, USA
 SO Polycyclic Aromatic Compounds (1999), 13(1), 79-92
 CODEN: PARCEO; ISSN: 1040-6638
 PB Gordon & Breach Science Publishers
 DT Journal
 LA English
 AB Fluorescence behavior of dicyclopenta[cd,fg]pyrene, dicyclopenta[cd,jk]pyrene and dicyclopenta[cd,mn]pyrene is reported in the presence of MeNO₂ and cetylpyridinium (CPy⁺) cation quenching agents. MeNO₂ and CPy⁺ are known to selectively quench fluorescence emission of alternant polycyclic aromatic hydrocarbons (PAHs). Emission intensities of nonalternant PAHs, with a few noted exceptions, are unaffected. Exptl. measurements show that MeNO₂ and CPy⁺ effectively quenched fluorescence emission of the 3 dicyclopentapyrenes, thus suggesting that the perimeter C:C double bonds in the 2 cyclopenta-rings are alkenic, rather than aromatic in nature. Also reported are the fluorescence properties of 14 aceanthrylene and acephenanthrylene derivs., as well as several structurally related compds., to further document the cetylpyridinium cation's quenching selectivity.
 CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
 Section cross-reference(s): 22
 IT 196-77-0, Benzo[def]cyclopenta[hi]chrysene 199-54-2, Benz[e]aceanthrylene 201-06-9, Acephenanthrylene 202-03-9, Aceanthrylene 208-96-8, Acenaphthylene 3343-10-0, 3-Methylbenz[j]aceanthrylene 7259-03-2 17057-80-6 18086-45-8 **19345-94-9**, 3-Methylacenaphthylene 19345-96-1 **19345-97-2**, 4-Methylacenaphthylene 19345-99-4, 1-Methylacenaphthylene 27208-37-3, Cyclopenta[cd]pyrene 39622-49-6 127229-46-3, Benz[j]aceanthrylene, 6-methyl-
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
 (fluorescence quenching of aceanthrylenes and acephenanthrylenes in cetylpyridinium chloride + cetyltrimethylammonium bromide micellar solns.)
 IT **19345-94-9**, 3-Methylacenaphthylene **19345-97-2**, 4-Methylacenaphthylene
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
 (fluorescence quenching of aceanthrylenes and acephenanthrylenes in cetylpyridinium chloride + cetyltrimethylammonium bromide micellar solns.)
 RN 19345-94-9 HCAPLUS
 CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)

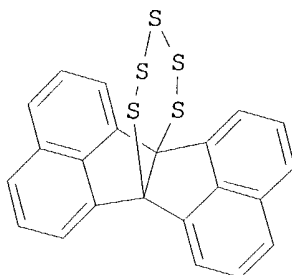


RN 19345-97-2 HCAPLUS
 CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

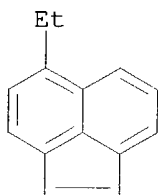
L53 ANSWER 7 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:197042 HCAPLUS
DN 130:311777
TI Synthesis of pentathiepanes and isolation of the conformers based on high
inversion barrier of the pentathiepane ring
AU Sugihara, Yoshiaki; Takeda, Hitoshi; Nakayama, Juzo
CS Department Chemistry, Faculty Science, Saitama University, Urawa, 338,
Japan
SO European Journal of Organic Chemistry (1999), (3), 597-605
CODEN: EJOCFK; ISSN: 1434-193X
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
OS CASREACT 130:311777
GI



I

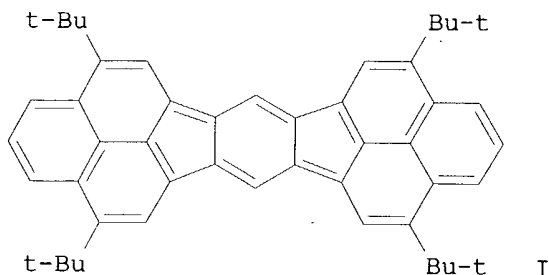
AB Acenaphtho[1,2-a]acenaphthylene was sulfurated with elemental S to give
pentathiepane I. A dynamic NMR spectrum anal. revealed that the 2
naphthalene rings of I are chemical nonequivalent $\leq 100^\circ$. The
pentathiepane ring of I adopts a chair conformation both in solution and
crystals. In accordance with NMR, the sulfuration of 5-
phenylacenaphtho[1,2-a]acenaphthylene gave a pair of conformers, which
were isolated in pure form. The Friedel-Crafts acetylation of I, followed
by dithioacetalization with HS(CH₂)₂SH, also gave a pair of isolable
conformers. These 2 pairs of conformers isomerized, as a result of the
ring inversion, to each other in solution at room temperature in the 1st-order
kinetics. The activation parameters for this process, E_a,
 $\Delta H_{thermod.}$, and $\Delta S_{thermod.}$, were determined Based on the exptl.
observations, a probable mechanism for the inversion process is proposed.
CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 22, 75

IT 10047-18-4P, 5-Acetylacenaphthene 13936-05-5P, 5-Ethylacenaphthene
 56252-14-3P 110864-35-2P 207606-15-3P 223518-14-7P
223518-16-9P 223518-23-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and conformation of pentathiepanes)
 IT **223518-16-9P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and conformation of pentathiepanes)
 RN 223518-16-9 HCAPLUS
 CN Acenaphthylene, 5-ethyl- (9CI) (CA INDEX NAME)



RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 8 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1998:150208 HCAPLUS
 DN 128:204534
 TI 4,8,12,16-Tetra-tert-butyl-s-indaceno[1,2,3-cd:5,6,7-c'd']diphenalene: a
 four-stage amphoteric redox system
 AU Ohashi, Kenji; Kubo, Takashi; Masui, Takashi; Yamamoto, Kageotoshi;
 Nakasuji, Kazuhiro; Takui, Takeji; Kai, Yasushi; Murata, Ichiro
 CS Department of Chemistry Graduate School of Science, Osaka University,
 Toyonaka, 560, Japan
 SO Journal of the American Chemical Society (1998), 120(9), 2018-2027
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 OS CASREACT 128:204534
 GI



AB A 4-stage amphoteric redox hydrocarbon (I) containing 2 phenalenyl units was
 prepared X-ray crystallog. of I reveals a delocalized D2h structure, which

is consistent with the presence of only 5 signals in the ^1H NMR spectrum of I at -60° . The cyclic voltammogram of I exhibits 4 reversible redox waves with a small numerical sum (Elsun) of 1st oxidation (Elox) and reduction (Elred) potentials. Four redox states of I were successfully generated from the neutral I, and were characterized by NMR, ESR and UV-visible-near-IR spectroscopies and theor. calcns. These spectral data reveal that phenalenyl units play an important role in the high amphotericity of I and the stability of the redox states generated.

CC 22-7 (Physical Organic Chemistry)

IT 203726-97-0P

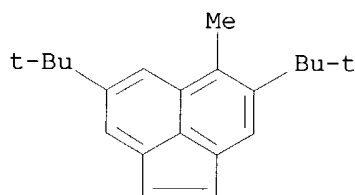
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(tetra-tert-butylindacenodiphenalene synthesis as four-stage amphoteric redox system)

IT 203726-97-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(tetra-tert-butylindacenodiphenalene synthesis as four-stage amphoteric redox system)

RN 203726-97-0 HCAPLUS

CN Acenaphthylene, 4,7-bis(1,1-dimethylethyl)-5-methyl- (9CI) (CA INDEX NAME)



RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 9 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:126870 HCAPLUS

DN 126:238774

TI A new method for chemical modification of conductive polypyrroles without destroying their conductivity

AU Ono, Noboru; Tsukamura, Chikanori; Nomura, Youta; Hironaga, Hideo; Murashima, Takashi; Ogawa, Takuji

CS Faculty Science, Ehime University, Matsuyama, 790, Japan

SO Advanced Materials (Weinheim, Germany) (1997), 9(2), 149-153

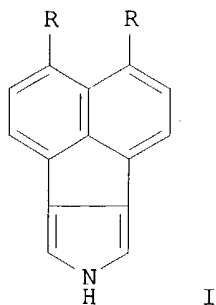
CODEN: ADVMEW; ISSN: 0935-9648

PB VCH

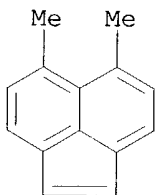
DT Journal

LA English

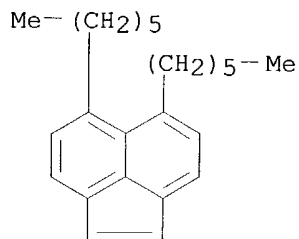
GI



- AB The electropolymn. of I (R = H, Cl, Me, n-C₆H₁₃) gave modified polypyrroles with electronic and phys. properties that could be controlled by varying R. The polymers have extended π -conjugation and good conductivity, which was not reduced by the introduction of substituents in the fused aromatic rings. I polymers showed a reversible and stable electrochromism, and were very stable in both the doped and undoped state. Also UV/VIS and fluorescence spectra of the polymers were measured.
- CC 35-7 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 36, 72, 73
- IT 208-96-8, Acenaphthylene 7267-09-6 **41002-83-9**
188240-45-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of pyrrole derivs. for electropolymn. to modified polypyrroles with retention of conductivity)
- IT 13132-28-0P, 1-Nitroacenaphthylene 144991-40-2P **188240-44-0P**
188240-46-2P **188240-47-3P** 188240-48-4P 188240-49-5P
188240-50-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of pyrrole derivs. for electropolymn. to modified polypyrroles with retention of conductivity)
- IT **41002-83-9 188240-45-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of pyrrole derivs. for electropolymn. to modified polypyrroles with retention of conductivity)
- RN 41002-83-9 HCAPLUS
- CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



- RN 188240-45-1 HCAPLUS
- CN Acenaphthylene, 5,6-diethyl- (9CI) (CA INDEX NAME)



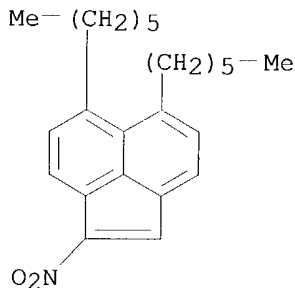
IT 188240-44-0P 188240-47-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of pyrrole derivs. for electropolymn. to modified polypyrroles with retention of conductivity)

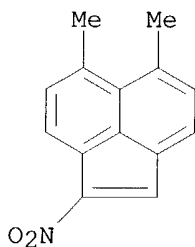
RN 188240-44-0 HCAPLUS

CN Acenaphthylene, 5,6-dihexyl-1-nitro- (9CI) (CA INDEX NAME)



RN 188240-47-3 HCAPLUS

CN Acenaphthylene, 5,6-dimethyl-1-nitro- (9CI) (CA INDEX NAME)



L53 ANSWER 10 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:46295 HCAPLUS

DN 126:173886

TI Diagenetic and catagenetic products of isorenieratene: molecular indicators for photic zone anoxia

AU Koopmans, Martin P.; Koster, Juergen; van Kaam-Peters, Heidi M. E.; Kenig, Fabien; Schouten, Stefan; Hartgers, Walter A.; de Leeuw, Jan W.; Damste, Jaap S. Sinninghe

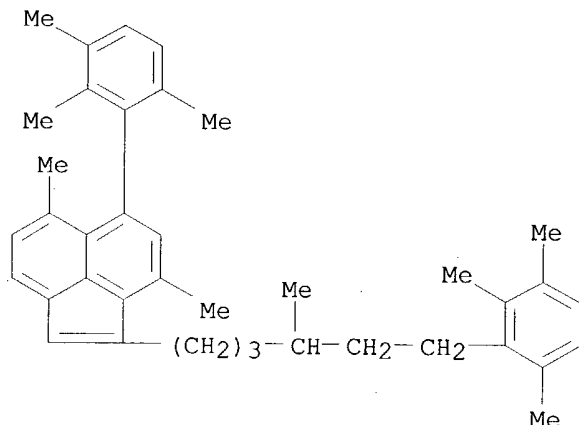
CS Dep. Marine Biogeochem. Toxicol., Netherlands Inst. Sea Res. (NIOZ), Den

- Burg, 1790 AB, Neth.
- SO Geochimica et Cosmochimica Acta (1996), 60(22), 4467-4496
CODEN: GCACAK; ISSN: 0016-7037
- PB Elsevier
- DT Journal
- LA English
- AB A wide range of novel diagenetic and catagenetic products of the diarom. carotenoid isorenieratene, a pigment of the photosynthetic green sulfur bacteria Chlorobiaceae, were identified in a number of sedimentary rocks ranging from Ordovician to Miocene. Atropisomers contain an axially chiral center which, in combination with other chiral centers, resulted in two or more diastereomers that can be separated on a normal GC column. Because Chlorobiaceae-derived biomass is enriched in ^{13}C , high ^{13}C contents of isorenieratene derivs. support their inferred origins. These derivs. include C40-, C33-, and C32-diaryl isoprenoids and short-chain aryl isoprenoids with addnl. aromatic and/or S-containing rings. C33 and C32 compds. are diagenetic products of C33 and C32 "carotenoids" formed from isorenieratene during early diagenesis through expulsion of toluene and m-xylene, resp. Cyclization of the polyene acyclic isoprenoid chain can proceed via an intramol. Diels-Alder reaction, followed by aromatization of the newly formed ring. Sulphurization is also an important process during early diagenesis, competing with expulsion and cyclization. The inherent presence of a conjugated double bond system in carotenoids implies that similar diagenetic and catagenetic reactions can occur with all carotenoids. Because Chlorobiaceae live at or below the oxic/anoxic boundary layer and require both light and H_2S , the presence of isorenieratene or its diagenetic and catagenetic products in ancient sedimentary rocks and crude petroleum is an excellent indication for photic zone anoxia in the depositional environment. Thus, these diagenetic and catagenetic products of isorenieratene can be used in reconstruction of palaeoenvironments and in oil-oil and oil-source rock correlation studies. Their presence in several petroleum source rocks suggested that anoxia is an important environmental parameter for the preservation of organic matter.
- CC 51-1 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 53, 61
- IT 153402-53-0 161269-47-2 187162-36-3 187162-38-5 187162-40-9
187162-42-1 187162-44-3 187162-46-5 187162-48-7 187162-50-1
187162-52-3 187162-54-5 187162-56-7 187162-58-9 **187162-60-3**
187162-62-5 187162-64-7 187162-66-9 187162-68-1 187162-70-5
187162-72-7 187162-74-9 187162-76-1 187162-78-3 187162-80-7
187162-83-0 187162-85-2 187162-87-4 187162-90-9 187162-92-1
187162-94-3 187162-96-5 187162-98-7 187163-00-4 187163-02-6
187163-04-8 187163-06-0 187163-08-2 187163-10-6 187163-12-8
187163-14-0 187163-16-2 187163-18-4 187163-20-8 187163-22-0
187163-24-2 187163-26-4 187163-28-6 187163-30-0 187163-32-2
187163-34-4 187163-36-6 187163-38-8 187163-39-9 187163-41-3
187163-44-6 187163-46-8 187163-48-0 187163-50-4 187163-52-6
187163-54-8 187163-56-0 187163-58-2 187163-60-6 187163-62-8
187163-64-0 187163-65-1 187163-66-2 187163-67-3 187163-68-4
187163-69-5 187163-70-8
- RL: GFM (Geological or astronomical formation); GOC (Geological or astronomical occurrence); GPR (Geological or astronomical process); FORM (Formation, nonpreparative); OCCU (Occurrence); PROC (Process)
(diagenetic and catagenetic products of isorenieratenes as biomarkers for photic zone anoxia in petroleum genesis)
- IT **187162-60-3**
RL: GFM (Geological or astronomical formation); GOC (Geological or astronomical occurrence); GPR (Geological or astronomical process); FORM

(Formation, nonpreparative); OCCU (Occurrence); PROC (Process)
(diagenetic and catagenetic products of isorenieratenes as biomarkers
for photic zone anoxia in petroleum genesis)

RN 187162-60-3 HCAPLUS

CN Acenaphthylene, 5,8-dimethyl-1-[4-methyl-6-(2,3,6-trimethylphenyl)hexyl]-6-(2,3,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



RE.CNT 124 THERE ARE 124 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 11 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:38495 HCAPLUS

DN 126:171182

TI Double-bond shifts in [4n]annulenes as a new principle for molecular switches. First results with dimethyl heptalene-1,2- and -4,5-dicarboxylates

AU Briquet, Anne Andree Sophie; Uebelhart, Peter; Hansen, Hans Juergen
CS Organisch-Chemisches Institut, Universitaet Zuerich, Zurich, CH-8057, Switz.

SO Helvetica Chimica Acta (1996), 79(8), 2282-2315

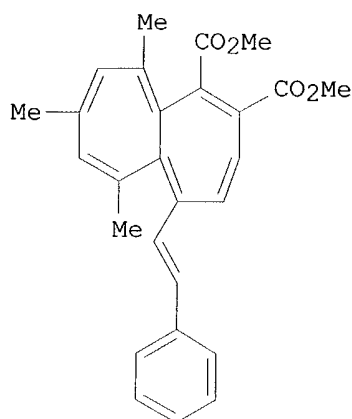
CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta

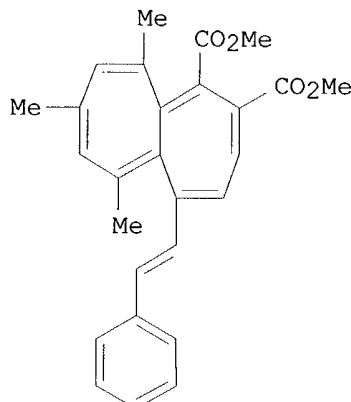
DT Journal

LA English

GI



I



II

AB A concept for mol. switches, based on thermal or photochem. double-bond shifts (DBS) in [4n]annulenes such as heptalenes or cyclooctatetraenes is introduced. Several heptalene-1,2- and -4,5-dicarboxylates with (E)-styryl and Ph groups at C(5) and C(1), or C(4) and C(2), resp., were investigated. X-ray crystal-structure anal. showed that the (E)-styryl group occupies in the crystals an almost perfect s-trans-conformation with respect to the C:C bond of the (E)-styryl moiety and the adjacent C:C bond of the heptalene core. Supplementary 1H-NOE measurements showed that the s-trans-conformations are also adopted in solution. Therefore, the DBS process in heptalenes is always accompanied by a 180° torsion of the (E)-styryl group with respect to its adjacent C:C bond of the heptalene core. UV/Vis spectra of the heptalene-1,2- and -4,5-dicarboxylates illustrated that it can be differentiated between an 'off-state', which possesses no 'through-conjugation' of the π -donor substituent and the corresponding MeO₂C group and an 'on-state' where this 'through-conjugation' is realized. The 'through-conjugation', i.e., conjugative interaction via the involved s-cis-butadiene substructure of the heptalene skeleton, is indicated by a strong enhancement of the intensities of the heptalene absorption bands I and II. The most impressive examples are the heptalenedicarboxylates I, representing the off-state, and II which stands for the on-state.

CC 22-6 (Physical Organic Chemistry)

Section cross-reference(s): 24, 25, 75

IT 58151-01-2P 186651-16-1P 186651-17-2P 186651-18-3P

186651-19-4P

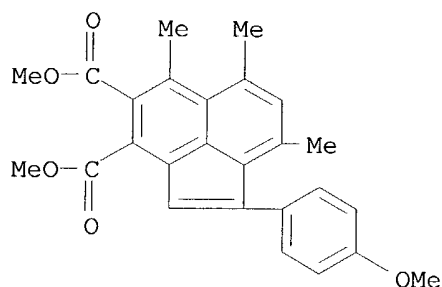
RL: BYP (Byproduct); PREP (Preparation)
(preparation of heptalenedicarboxylates)

IT **186651-19-4P**

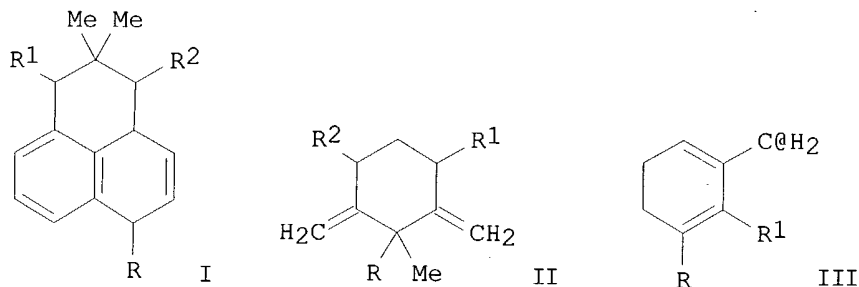
RL: BYP (Byproduct); PREP (Preparation)
(preparation of heptalenedicarboxylates)

RN 186651-19-4 HCAPLUS

CN 3,4-Acenaphthylenedicarboxylic acid, 1-(4-methoxyphenyl)-5,6,8-trimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



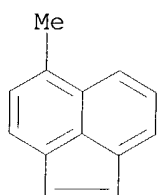
L53 ANSWER 12 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:743463 HCAPLUS
 DN 126:131099
 TI Resonance energy of diradicals. 1,8-Naphthoquinodimethane
 AU Roth, Wolfgang R.; Unger, Christian; Wasser, Thorsten
 CS Fakultät Chemie, Universitaet Bochum, Bochum, D-44780, Germany
 SO Liebigs Annalen (1996), (12), 2155-2169
 CODEN: LANAEM; ISSN: 0947-3440
 PB VCH
 DT Journal
 LA German
 GI



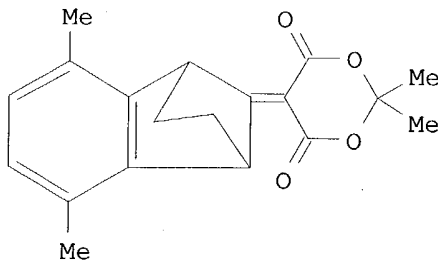
AB From the racemization of methanoacenaphthylene I ($R = \text{Me}$, $R_1R_2 = \text{bond}$) and the temperature and NO dependence of the trapping rate of perinaphthadiyl I ($R = \text{H}$; $R_1, R_2 = \text{electron}$) between 218 and 288° the energy profile for the equilibrium I ($R = \text{H}$, $R_1R_2 = \text{bond}$) was derived. The singlet-triplet splitting of the diradical is 2.5 kcal·mol⁻¹ with the triplet being the ground state. By comparison of the exptl. reaction enthalpy with the analogous value for bicyclohexane II ($R = \text{Me}$, Et ; $R_1R_2 = \text{bond}$), diradical II ($R = \text{Me}$, Et ; $R_1, R_2 = \text{electron}$) or a hypothetical model reaction with non-interacting radicals the stabilizing interaction of the radicals in the singlet state of I ($R = \text{H}$; $R_1, R_2 = \text{electron}$) is negligible making the stabilization of the triplet equivalent to the singlet-triplet splitting. By using literature data it is shown by an analogous anal. that the interaction of the radicals in the bisallyl diradical III ($R = \text{H}$, $R_1 = \text{C}\bullet\text{H}_2$) and in the triplet state of III ($R = \text{C}\bullet\text{H}_2$, $R_1 = \text{H}$) is also negligible whereas in the singlet state of III ($R = \text{C}\bullet\text{H}_2$, $R_1 = \text{H}$) the interaction is strongly destabilizing.

CC 22-6 (Physical Organic Chemistry)

Section cross-reference(s): 25
 IT 1193-55-1P, 2-Methyl-1,3-cyclohexanedione 19335-98-9P 19345-88-1P
19345-91-6P 19565-21-0P 25112-82-7P 25178-74-9P
 41791-10-0P 186349-16-6P 186349-19-9P 186349-26-8P 186349-32-6P
 186349-33-7P 186352-69-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (resonance energy of naphthoquinodimethane diradicals)
 IT **19345-91-6P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (resonance energy of naphthoquinodimethane diradicals)
 RN 19345-91-6 HCAPLUS
 CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 13 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1994:700262 HCAPLUS
 DN 121:300262
 TI Conversion of 5-(4,7-dimethyl-1,3-dihydro-1,3-ethano-2H-inden-2-ylidene)-
 2,2-dimethyl-1,3-dioxan-4,6-dione into 3-methylacenaphthylene in a flash
 vacuum pyrolytic experiment
 AU Bell, Stephanie E. V.; Brown, Roger F. C.; Coulston, Karen J.; Eastwood,
 Frank W.
 CS Chemistry Department, Monash University, Clayton, 3168, Australia
 SO Australian Journal of Chemistry (1994), 47(8), 1469-81
 CODEN: AJCHAS; ISSN: 0004-9425
 DT Journal
 LA English
 GI



I

AB Flash vacuum pyrolysis of 5-(4,7-dimethyl-1,3-dihydro-1,3-ethano-2H-inden-
 2-ylidene)-2,2-dimethyl-1,3-dioxan-4,6-dione (I) at temps. in the range
 600-750° led to complex mixts., but at higher temps. (850°)

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it was converted into 3-methylacenaphthylene (major) and 1,4-dimethylnaphthalene (minor). 5-Ethenyl-1,4-dimethylnaphthalene on f.v.p. at 850° gave 5-methylacenaphthylene together with other compds. and was not on the reaction pathway.

CC 22-4 (Physical Organic Chemistry)

Section cross-reference(s): 25

IT **19345-91-6P**, 5-Methylacenaphthylene **19345-94-9P**,
3-Methylacenaphthylene 88916-64-7P, 5-Ethenyl-1,4-dimethylnaphthalene
159263-64-6P 159263-65-7P 159263-66-8P 159263-69-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(study of pyrolysis/carbene rearrangement of (ethanoindenylidene)-1,3-dioxanedione)

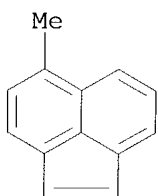
IT **19345-91-6P**, 5-Methylacenaphthylene **19345-94-9P**,
3-Methylacenaphthylene

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(study of pyrolysis/carbene rearrangement of (ethanoindenylidene)-1,3-dioxanedione)

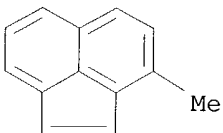
RN 19345-91-6 HCAPLUS

CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-94-9 HCAPLUS

CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 14 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1994:579005 HCAPLUS

DN 121:179005

TI Some physical properties of methyl derivatives of o-pleiadienequinones

AU Ohashi, Akihiro; Aida, Takashi; Tsunetsugu, Josuke

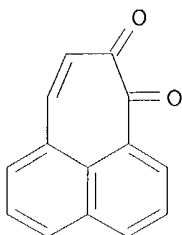
CS Department of Chemistry, Faculty of Science, Saitama University, Urawa,
338, Japan

SO Journal of Molecular Structure (1994), 324(1-2), 75-82
CODEN: JMOSB4; ISSN: 0022-2860

DT Journal

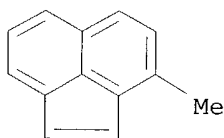
LA English

GI

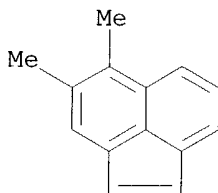


I

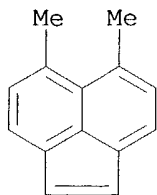
- AB Spectral (UV, IR, mass, ¹H and ¹³C NMR) and electrochem. properties of o-pleiadienequinone (I) and its Me derivs. are described. Heats of formation are calculated by the MNDO-PM3 method.
- CC 22-10 (Physical Organic Chemistry)
Section cross-reference(s): 72
- IT **19345-94-9P**, 3-Methylacenaphthylene **41002-81-7P**,
4,5-Dimethylacenaphthylene **41002-83-9P**, 5,6-Dimethylacenaphthylene **41082-61-5P**, 3,7-Dimethylacenaphthylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cycloaddn. reaction with dichloroketene)
- IT **19345-94-9P**, 3-Methylacenaphthylene **41002-81-7P**,
4,5-Dimethylacenaphthylene **41002-83-9P**, 5,6-Dimethylacenaphthylene **41082-61-5P**, 3,7-Dimethylacenaphthylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cycloaddn. reaction with dichloroketene)
- RN 19345-94-9 HCAPLUS
- CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



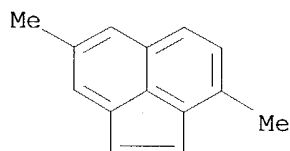
- RN 41002-81-7 HCAPLUS
- CN Acenaphthylene, 4,5-dimethyl- (9CI) (CA INDEX NAME)



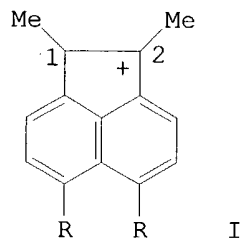
- RN 41002-83-9 HCAPLUS
- CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



RN 41082-61-5 HCAPLUS
 CN Acenaphthylene, 3,7-dimethyl- (9CI) (CA INDEX NAME)

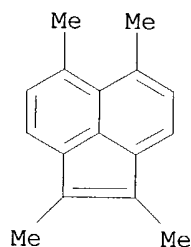


L53 ANSWER 15 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1991:582355 HCAPLUS
 DN 115:182355
 TI General structure-reactivity relationships for 1,2-hydrogen shifts in carbocations and neutral compounds
 AU Borodkin, G. I.; Susharin, E. R.; Elanov, I. R.; Shakirov, M. M.; Shubin, V. G.
 CS Novosib. Inst. Org. Khim., Novosibirsk, USSR
 SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1991), (6), 1352-8
 CODEN: IASKA6; ISSN: 0002-3353
 DT Journal
 LA Russian
 GI

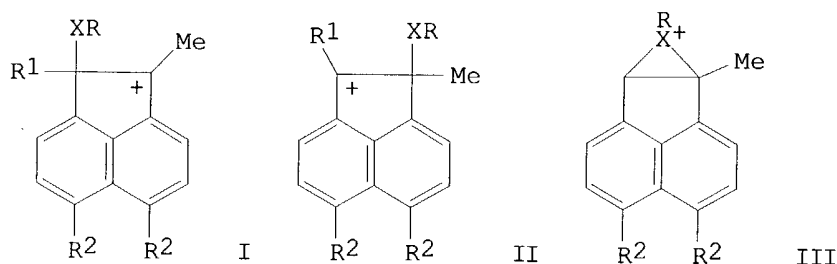


AB Linear equations correlating the activation parameters for degenerate 1,2 H shift in acenaphthylenonium ions I (R = Me, Br) with chemical shift of the carbonium-ion C or other measures of electron deficit - total or π -electron charge at the carbonium C calculated by CNDO/2 - were established.
 CC 22-6 (Physical Organic Chemistry)
 IT 132118-72-0 132118-73-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (protonation of, in superacid, carbonium ion by)
 IT **132118-73-1**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (protonation of, in superacid, carbonium ion by)
 RN 132118-73-1 HCAPLUS
 CN Acenaphthylene, 1,2,5,6-tetramethyl- (9CI) (CA INDEX NAME)



L53 ANSWER 16 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1991:100774 HCAPLUS
 DN 114:100774
 TI Stereoelectronic aspects of the interaction between reagents RXCl (X = sulfur, selenium) and acenaphthylene derivatives in superacids
 AU Borodkin, G. I.; Chernyak, E. I.; Shakirov, M. M.; Shubin, V. G.
 CS Novosib. Inst. Org. Khim., Novosibirsk, USSR
 SO Metalloorganicheskaya Khimiya (1990), 3(5), 1017-24
 CODEN: MEKHEX; ISSN: 0235-0114
 DT Journal
 LA Russian
 GI



AB Substituent effects on the relative equilibrium stability of acynaphthylenonium ions I, II and π -complex III (RX = MeS, C₆H₅S, C₆F₅S, C₆H₅Se, C₆F₅Se, OH, Br; R1 = Me, CH₂Cl; R2 = H, Br, Me) were studied by NMR. The relative contribution of III falls with increasing atomic number of X, electron-donor character of R1, and electron-accepting character of R2. In several of the episulfonium ions III, trans stereochem. of the R and R1 groups was established by NMR and interpreted as a steric effect; the absence of temperature effect on the NMR indicated that these trans isomers were static, and that a rapid equilibrium with minor concentration of the cis isomer is not

involved. MINDO/3 calcns. on the potential energy surface of III are reported as well.

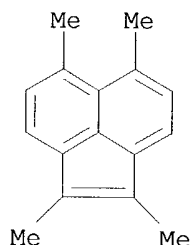
CC 22-4 (Physical Organic Chemistry)

IT 132118-72-0P **132118-73-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and conversion of, to acynaphthylenonium ion)

IT **132118-73-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and conversion of, to acynaphthylenonium ion)

RN 132118-73-1 HCAPLUS

CN Acenaphthylene, 1,2,5,6-tetramethyl- (9CI) (CA INDEX NAME)



L53 ANSWER 17 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:575325 HCAPLUS

DN 113:175325

TI Hydropyrolysis of coal. Influence of temperature and hydrogen pressure on the yield and composition of hydropyrolysis tars

AU Kaernbach, W.; Dyla, P.; Zobel, H.

CS Inst. Coal Chem., Pol. Acad. Sci., Gliwice, Pol.

SO Erdoel & Kohle, Erdgas, Petrochemie (1990), 43(7/8), 291-4
 CODEN: EKEPAB; ISSN: 0014-0058

DT Journal

LA German

AB The influence of reaction conditions on the hydropyrolysis of Polish hard coals is described. The yield of the main products and the composition of the structure types of the hydropyrolysis tars were studied by TGA and gas chromatog. The hydropyrolysis was carried out in a fixed-bed pressure reactor. The optimal reaction conditions were at 873 K and 3 MPa H pressure.

CC 51-21 (Fossil Fuels, Derivatives, and Related Products)

IT 71-43-2P, Benzene, preparation 90-12-0P, 1-Methylnaphthalene 91-20-3P, Naphthalene, preparation 91-57-6P, 2-Methylnaphthalene 92-52-4P, 1,1'-Biphenyl, preparation 95-47-6P, preparation 95-63-6P, 1,2,4-Trimethylbenzene 100-41-4P, Ethylbenzene, preparation 106-42-3P, p-Xylene, preparation 108-38-3P, m-Xylene, preparation 108-67-8P, 1,3,5-Trimethylbenzene, preparation 108-88-3P, preparation 111-65-9P, N-Octane, preparation 111-66-0P, 1-Octene 111-84-2P, Nonane 112-40-3P, n-Dodecane 112-41-4P, 1-Dodecene 112-88-9P, 1-Octadecene 112-95-8P, n-Eicosane 124-11-8P, 1-Nonene 124-18-5P, n-Decane 142-82-5P, n-Heptane, preparation 496-11-7P, Indan 526-73-8P, 1,2,3-Trimethylbenzene 538-68-1P, Pentylbenzene 544-76-3P, n-Hexadecane 571-58-4P, 1,4-Dimethylnaphthalene 573-98-8P, 1,2-Dimethylnaphthalene 575-37-1P, 1,7-Dimethylnaphthalene 575-41-7P, 1,3-Dimethylnaphthalene 575-43-9P, 1,6-Dimethylnaphthalene 581-40-8P, 2,3-Dimethylnaphthalene 581-42-0P, 2,6-Dimethylnaphthalene 582-16-1P, 2,7-Dimethylnaphthalene 593-45-3P, n-Octadecane 593-49-7P,

n-Heptacosane 629-50-5P, n-Tridecane 629-59-4P, n-Tetradecane 629-62-9P, Pentadecane 629-78-7P, n-Heptadecane 629-92-5P, n-Nonadecane 629-94-7P, n-Heneicosane 629-97-0P, n-Docosane 629-99-2P, n-Pentacosane 630-01-3P, n-Hexacosane 630-02-4P, n-Octacosane 630-03-5P, n-Nonacosane 630-04-6P, n-Hentriacontane 638-67-5P, n-Tricosane 638-68-6P, n-Triacontane 641-91-8P, 1,2,5-Trimethylnaphthalene 646-31-1P, n-Tetracosane 767-58-8P, 1-Methylindan 821-95-4P, 1-Undecene 824-22-6P, 4-Methylindan 824-63-5P, 2-Methylindan 829-26-5P, 2,3,6-Trimethylnaphthalene 872-05-9P, 1-Decene 874-35-1P, 5-Methylindan 939-27-5P, 2-Ethylnaphthalene 1120-21-4P, Undecane 1127-76-0P, 1-Ethylnaphthalene 1320-27-0P, Pentylnaphthalene 1599-67-3P, 1-Docosene 1680-51-9P, 1685-83-2P, 2131-38-6P, 1,3,7-Trimethylnaphthalene 2131-39-7P, 1,3,5-Trimethylnaphthalene 2131-42-2P, 1,4,6-Trimethylnaphthalene 2245-38-7P, 2,3,5-Trimethylnaphthalene 2437-56-1P, 1-Tridecene 2717-42-2P, 1,2,4-Trimethylnaphthalene 2809-64-5P 3031-08-1P, 1,3,6-Trimethylnaphthalene 4471-17-4P, Methyldiphenyl 13556-58-6P 18435-45-5P, 1-Nonadecene **19345-91-6P 19345-94-9P 19345-97-2P** 26266-05-7P, n-Heptadecene 26916-61-0P 26952-13-6P, n-Tetradecene 26952-14-7P, n-Hexadecene 27251-68-9P, n-Pentadecene 27378-74-1P, Propylnaphthalene 27400-78-8P, n-Eicosene 27400-79-9P, n-Heneicosene 31324-50-2P 31391-42-1P 31711-50-9P, Butylnaphthalene 36541-18-1P, Trimethylindan 51855-29-9P 53563-67-0P, Dimethylindan 56924-46-0P, n-Tricosene 66256-38-0P, 4-Ethylindan 95012-76-3P 95676-53-2P 108114-27-8P 130004-87-4P 130004-89-6P 130005-08-2P

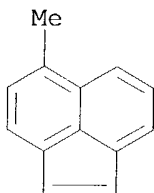
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in hydropyrolysis tars of Polish coal)

IT **19345-91-6P 19345-94-9P 19345-97-2P**

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in hydropyrolysis tars of Polish coal)

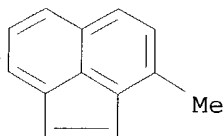
RN 19345-91-6 HCAPLUS

CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



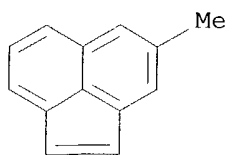
RN 19345-94-9 HCAPLUS

CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)

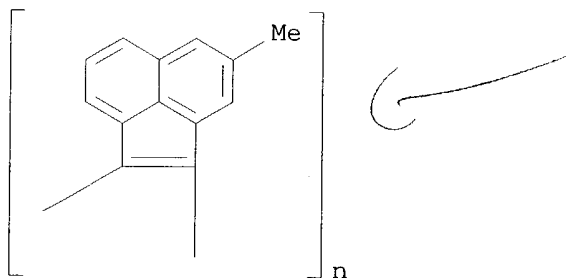


RN 19345-97-2 HCAPLUS

CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 18 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1987:637616 HCAPLUS
 DN 107:237616
 TI Structure and properties of nonclassical polymers. V. On a class of nonalternant polymers with localized nonbonding bands
 AU Polansky, O. E.; Schuster, P.; Ivanov, Ts.; Tyutyulkov, N.
 CS Max-Planck-Inst. Strahlenchem., Muelheim an der Ruhr, D-4330, Fed. Rep. Ger.
 SO International Journal of Quantum Chemistry (1987), 32(4), 491-9
 CODEN: IJQCB2; ISSN: 0020-7608
 DT Journal
 LA English
 AB Nonclassical, extended polymeric hydrocarbon networks exhibiting localized, infinitely narrow nonbonding bands (NBMO) owing to different structural peculiarities were studied, and proof of the rigorous localization of the occurring NBMOs was provided. The possible ferromagnetic alignment originating from the spin correlation in this band is discussed. A specific relevance of the Coulson-Rushbrock theorem to nonalternant polymers was realized on the basis of the structural principles formulated, which included dividing the monomeric unit into a nonclassical alternant fragment (Q) (e.g., pentadienyl) and a classical subunit (R) (e.g., ethene) and bridging the Q subunits with R subunits.
 CC 36-2 (Physical Properties of Synthetic High Polymers)
 Section cross-reference(s): 65, 77
 IT 111763-22-5 111763-23-6 **111763-24-7**
 RL: PRP (Properties)
 (with localized nonbonding bands, band structure and magnetic order in relation to)
 IT **111763-24-7**
 RL: PRP (Properties)
 (with localized nonbonding bands, band structure and magnetic order in relation to)
 RN 111763-24-7 HCAPLUS
 CN Poly(4-methyl-1,2-acenaphthylenediyl) (9CI) (CA INDEX NAME)



L53 ANSWER 19 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

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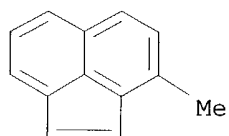
AN 1987:181789 HCAPLUS
 DN 106:181789
 TI Identification of organic compounds produced during combustion of a polymer mixture
 AU Hawley-Fedder, R. A.; Parsons, M. L.; Karasek, F. W.
 CS Lawrence Livermore Natl. Lab., Livermore, CA, 94550, USA
 SO Journal of Chromatography (1987), 387, 207-21
 CODEN: JOCRAM; ISSN: 0021-9673
 DT Journal
 LA English
 AB A mixture containing polyethylene [9002-88-4], polystyrene [9003-53-6], and poly(vinyl chloride) [9002-86-2] was subjected to oxidative thermal degradation at temps. of 800-950°. Break-down products were collected on glass wool or in cold traps for anal. by capillary gas chromatog. and gas chromatog.-mass spectrometry. Combustion products included alkyl benzenes, hydrocarbons, alkenes, biphenyls, and polycyclic aromatic hydrocarbons containing 2-6 rings.

CC 59-2 (Air Pollution and Industrial Hygiene)
 Section cross-reference(s): 35, 38, 60

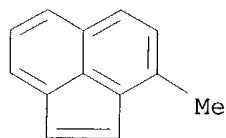
IT 56-49-5P, 3-Methylcholanthrene 56-55-3P, Benzo[a]anthracene 84-15-1P, o-Terphenyl 85-01-8P, preparation 86-73-7P, Fluorene 90-12-0P, 1-Methylnaphthalene 91-20-3P, preparation 91-57-6P, 2-Methylnaphthalene 92-06-8P, m-Terphenyl 92-24-0P, Naphthacene 92-52-4P, preparation 92-94-4P, p-Terphenyl 95-13-6P 98-82-8P, Cumene 100-42-5P, preparation 100-80-1P, m-Methylstyrene 101-81-5P, Diphenylmethane 103-65-1P, Propylbenzene 120-12-7P, Anthracene, preparation 129-00-0P, preparation 135-48-8P, Pentacene 191-24-2P, Benzo[ghi]perylene 191-26-4P, Dibenzo[def,mno]chrysene 195-19-7P, Benzo[c]phenanthrene 203-12-3P, Benzo[ghi]fluoranthene 203-64-5P, 4,5-Methylenephenanthrene 203-80-5P 206-44-0P, Fluoranthene 208-96-8P, Acenaphthylene 213-46-7P, Picene 215-58-7P, Dibenz[a,c]anthracene 217-59-4P, Triphenylene 218-01-9P, Chrysene 275-51-4P, Azulene 300-57-2P, 3-Phenylpropene 496-11-7P, Indane 501-65-5P, Diphenylacetylene 530-48-3P, 1,1-Diphenylethene 575-41-7P, 1,3-Dimethylnaphthalene 588-59-0P 604-53-5P, 1,1'-Binaphthyl 605-02-7P, 1-Phenylnaphthalene 610-48-0P, 1-Methylantracene 611-15-4P, o-Methylstyrene 611-45-0P, 1-Benzyl-naphthalene 612-78-2P, 2,2'-Binaphthyl 612-94-2P, 2-Phenylnaphthalene 613-31-0P, Dihydroanthracene 622-97-9P, p-Methylstyrene 637-50-3P, 1-Propenylbenzene 643-58-3P, 2-Methylbiphenyl 643-93-6P, 3-Methylbiphenyl 644-08-6P, 4-Methylbiphenyl 826-74-4P, 1-Vinylnaphthalene 827-54-3P, 2-Vinylnaphthalene 832-71-3P, 3-Methylphenanthrene 883-20-5P, 9-Methylphenanthrene 939-27-5P, 2-Ethylnaphthalene 1081-75-0P, 1,3-Diphenylpropane 1127-76-0P, 1-Ethylnaphthalene 1430-97-3P, 2-Methylfluorene 1730-37-6P, 1-Methylfluorene 2381-21-7P, 1-Methylpyrene 2489-87-4P 2498-75-1P 2498-77-3P 2523-37-7P, 9-Methylfluorene 2871-91-2P 3351-30-2P, 4-Methylchrysene 4325-74-0P, 1,2'-Binaphthyl 4325-76-2P, 1-Phenylphenanthrene 6111-78-0P **19345-94-9P**, 3-Methylacenaphthylene 19345-99-4P, 1-Methylacenaphthylene 25323-41-5P, Chloroxylene 25550-14-5P, Methyleneethylbenzene 26856-35-9P, Dihydrophenanthrene 28700-83-6P 29036-02-0P, Quaterphenyl 30777-18-5P, Benzo[a]fluorene 30777-19-6P, Benzo[b]fluorene 30900-94-8P 38620-92-7P, Benzyl-naphthalene 56832-73-6P, Benzofluoranthene 66161-17-9P 73467-76-2P, Benzopyrene 107843-54-9P 108115-36-2P

RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, in combustion of polyethylene-polystyrene-poly(vinyl chloride) mixts., waste incineration in relation to)

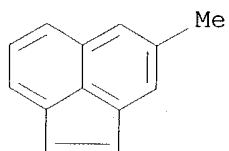
IT **19345-94-9P**, 3-Methylacenaphthylene
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, in combustion of polyethylene-polystyrene-poly(vinyl chloride) mixts., waste incineration in relation to)
 RN 19345-94-9 HCAPLUS
 CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



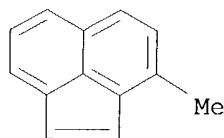
L53 ANSWER 20 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1985:154078 HCAPLUS
 DN 102:154078
 TI Products obtained during combustion of polymers under simulated incinerator conditions. III. Poly(vinyl chloride)
 AU Hawley-Fedder, R. A.; Parsons, M. L.; Karasek, F. W.
 CS Dep. Chem., Arizona State Univ., Tempe, AZ, 85287, USA
 SO Journal of Chromatography (1984), 315, 211-21
 CODEN: JOCRAM; ISSN: 0021-9673
 DT Journal
 LA English
 AB Combustion products from poly(vinyl chloride) [9002-86-2] were determined using gas chromatog. and gas chromatog.-mass spectrometry. Combustion conditions were 800-950°, and an attempt was made to approx. municipal incinerator conditions. Compds. identified consisted of PAHs and alkylbenzenes. Two chlorinated species were identified.
 CC 59-4 (Air Pollution and Industrial Hygiene)
 Section cross-reference(s): 38
 IT 50-32-8P, preparation 56-49-5P 56-55-3P 71-43-2P, preparation
 85-01-8P, preparation 86-73-7P 90-12-0P 91-20-3P, preparation
 91-57-6P 92-52-4P, preparation 92-94-4P 95-13-6P 103-65-1P
 108-95-2P, preparation 120-12-7P, preparation 129-00-0P, preparation
 135-48-8P 191-24-2P 192-97-2P 195-19-7P 198-55-0P 203-12-3P
 203-64-5P 203-80-5P 206-44-0P 208-96-8P 213-46-7P 218-01-9P
 275-51-4P 501-65-5P 571-58-4P 575-41-7P 581-40-8P 581-42-0P
 605-02-7P 612-94-2P 613-12-7P 643-93-6P 644-08-6P 826-74-4P
 827-54-3P 883-20-5P 886-66-8P 1127-76-0P 1430-97-3P 1576-69-8P
 1705-85-7P 1730-37-6P 2381-21-7P 2381-31-9P 2417-82-5P
 2498-77-3P 2871-91-2P 3287-02-3P 3351-31-3P 4325-76-2P
 6111-78-0P 6268-37-7P 17088-22-1P **19345-94-9P**
19345-97-2P 19345-99-4P 25323-41-5P 26856-35-9P
 30777-18-5P 30777-19-6P 42862-12-4P 53571-97-4P 56832-73-6P
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, from polyvinyl chloride incineration)
 IT **19345-94-9P 19345-97-2P**
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, from polyvinyl chloride incineration)
 RN 19345-94-9 HCAPLUS
 CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-97-2 HCAPLUS
CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)

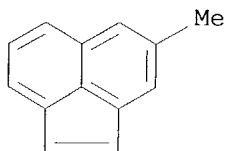


L53 ANSWER 21 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:66681 HCAPLUS
DN 102:66681
TI Products obtained during combustion of polymers under simulated incinerator conditions. I. Polyethylene
AU Hawley-Fedder, R. A.; Parsons, M. L.; Karasek, F. W.
CS Dep. Chem., Arizona State Univ., Tempe, AZ, 85287, USA
SO Journal of Chromatography (1984), 314, 263-73
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB An apparatus permitting the combustion of large (2 g) polymer samples at high temperature is described. Effluents from combustion are collected in cold traps
(liquid N) and on glass wool for anal. by capillary gas chromatog. and gas chromatog.-mass spectrometry. Products from polyethylene [9002-88-4] combustion at 800, 850, 900, and 950° are determined
CC 59-4 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 38
IT 19345-94-9 19345-97-2 19345-99-4 30777-18-5
30777-19-6 35465-71-5
RL: OCCU (Occurrence)
(in polyethylene incineration combustion products)
IT 19345-94-9 19345-97-2
RL: OCCU (Occurrence)
(in polyethylene incineration combustion products)
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-97-2 HCAPLUS

CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 22 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1982:438636 HCAPLUS
 DN 97:38636
 TI Anomalous Leuckart reaction of acenaphthenones. II. Anomalous Leuckart reaction of 3-methyl- and 5-methyl-1-acenaphthenones
 AU Tatsugi, Jiro; Okumura, Michio
 CS Dep. Appl. Chem., Aichi Inst. Technol., Toyota, 470-03, Japan
 SO Nippon Kagaku Kaishi (1982), (5), 876-9
 CODEN: NKA KB8; ISSN: 0369-4577
 DT Journal
 LA Japanese
 OS CASREACT 97:38636
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Methylacenaphthenone isomers (I; R = Me, R1 = H, R1 = H, R = H, R1 = Me) gave anomalous Leuckart reaction products II and III, together with formylamino derivs. (IV). The aldol-type condensation products (V) were obtained from I (R = R1 = H; R = H, R1 = Me) but not from I (R = Me, R1 = H).

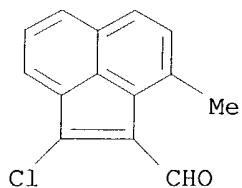
CC 25-26 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **58231-30-4P** 82318-84-1P 82318-85-2P 82318-86-3P
 82318-87-4P 82318-88-5P 82318-89-6P 82325-54-0P **82375-05-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

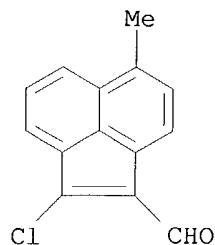
IT **58231-30-4P 82375-05-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 58231-30-4 HCAPLUS

CN 1-Acenaphthylenecarboxaldehyde, 2-chloro-8-methyl- (9CI) (CA INDEX NAME)

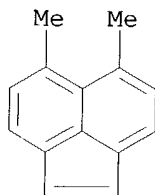


RN 82375-05-1 HCAPLUS
 CN 1-Acenaphthylenecarboxaldehyde, 2-chloro-6-methyl- (9CI) (CA INDEX NAME)



L53 ANSWER 23 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1981:588459 HCAPLUS
 DN 95:188459
 TI Radiation-resistant polymer compositions
 PA Japan Atomic Energy Research Institute, Japan; Furukawa Electric Co., Ltd.
 SO Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 56084748	A2	19810710	JP 1979-161570	19791214
	JP 61011263	B4	19860402		
PRAI	JP 1979-161570		19791214		
AB	Thermoplastic and rubber compns. with improved radiation resistance contain a C1-4 alkyl- or haloacenaphthylene and/or a haloindene ≥ 0.5 , a hydroperoxide 0.2-10, and an organic peroxide 0.5-10 phr. For example, a vulcanizate from 60:40 ethylene-propene rubber 100, Nocrack 224 0.5, S 0.1, clay 100, dicumyl peroxide 1, tert-Bu hydroperoxide 3, and 5,6-dimethylacenaphthylene (I) [41002-83-9] 3 parts had tensile strength 0.66 kg/mm ² (0.69 kg/mm ² after 100 Mrads γ -ray irradiation) and elongation 690 (610)%, compared with 0.65 (0.45) and 680 (140), resp., for a control not containing I.				
IC	C08L101-00; C08K005-01; C08K005-03; C08K005-14				
CC	38-9 (Elastomers, Including Natural Rubber)				
IT	41002-83-9				
	RL: USES (Uses)				
	(ethylene-propene rubber containing, radiation-resistant)				
IT	41002-83-9				
	RL: USES (Uses)				
	(ethylene-propene rubber containing, radiation-resistant)				
RN	41002-83-9 HCAPLUS				
CN	Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)				



L53 ANSWER 24 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1981:588151 HCAPLUS
 DN 95:188151
 TI Fireproofing of polymers
 PA Japan Atomic Energy Research Institute, Japan; Furukawa Electric Co., Ltd.
 SO Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

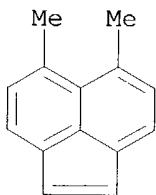
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 56084731	A2	19810710	JP 1979-161572	19791214
	JP 60015655	B4	19850420		
PRAI	JP 1979-161572		19791214		

AB Loss of strength in fireproofing of polymers with halogen compds. is reduced by crosslinking the fireproofed polymers with >0.5 phr acenaphthylene, optionally containing Cl-4 alkyl or halogen groups, or chlorinated or brominated indenenes. For example, a 1-mm sheet of polyethylene [9002-88-4] 100, Nocrack 300 0.3, (C6Br5)20 [1163-19-5] 30, Sb2O3 10, and 5,6-dimethylacenaphthylene (I) [41002-83-9] 10 parts was irradiated with 20 Mrad electron beams to give a crosslinked sheet with tensile strength 1.51 kg/mm², elongation 360%, and O index 25.5, compared with 1.22, 290, and 24.0, resp., without I, and 2.27, 480, and 19.0, resp., for polyethylene containing 0.3 phr Nocrack 300.

IC C08J007-12; C08K005-01; C08K005-03; C08L101-00
 CC 36-6 (Plastics Manufacture and Processing)
 IT **41002-83-9**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (crosslinking by, of fireproofed polyethylene for strength retention)

IT **41002-83-9**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (crosslinking by, of fireproofed polyethylene for strength retention)

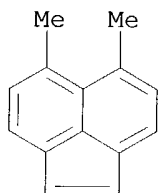
RN 41002-83-9 HCAPLUS
 CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



L53 ANSWER 25 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1981:570432 HCAPLUS
 DN 95:170432
 TI Chlorine-containing resin compositions
 PA Japan Atomic Energy Research Institute, Japan; Furukawa Electric Co., Ltd.
 SO Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI JP 56084730 A2 19810710 JP 1979-161571 19791214
 JP 60014779 B4 19850416
 PRAI JP 1979-161571 19791214
 AB Cl-containing polymers modified with ≥ 0.5 phr Cl-4 alkyl or halo acenaphthalenes and/or haloindenes under electron beam irradiation showed reduced HCl evolution in combustion. Thus, a 1 mm sheet from PVC [9002-86-2] 100, DOP 50, tribase 5, dibasic Pb stearate 0.3, CaCO₃ 70, and 5,6-dimethylacenaphthylene (I) [41002-83-9] 5 parts was irradiated with 15 Mrads electron beam to give a specimen with tensile strength 1.53 kg/mm², elongation 260%, tensile strength retention (after 4 h in 70° oil) 94%, elongation retention 83%, and HCl evolution 60 mg/g, compared with 2.10, 350, 105, 90, and 285, resp., for a control without I and the irradiation and 1.10, 170, 73, 53, and 60, resp., for a control without I, but with the irradiation
 IC C08J007-12; C08K003-22; C08K003-26; C08K005-01
 CC 36-6 (Plastics Manufacture and Processing)
 IT 41002-83-9
 RL: USES (Uses)
 (PVC containing, electron beam-irradiated, with improved hydrogen chloride evolution resistance)
 IT 41002-83-9
 RL: USES (Uses)
 (PVC containing, electron beam-irradiated, with improved hydrogen chloride evolution resistance)
 RN 41002-83-9 HCAPLUS
 CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



L53 ANSWER 26 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1981:498826 HCAPLUS

DN 95:98826

TI Fireproofing agents

PA Japan Atomic Energy Research Institute, Japan

SO Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 56016511	A2	19810217	JP 1979-92019	19790719
	JP 58001146	B4	19830110		
	US 4289687	A	19810915	US 1980-114420	19800122
PRAI	JP 1979-4802		19790122		
	JP 1979-92019		19790719		
AB	A fire-resistant resin composition contains an acenaphthylene derivative with				
2-7	Cl and/or Br atoms and 1-4 Cl-4 alkyl, alkoxy, and/or alkyl ester groups,				

and is treated to generate free radicals. Thus, to polyethylene (I) (ZF-30) [9002-88-4] 100, chlorinated I (Cl content 40%) 35, 3-methyl-1,5,6,8-tetrabromoacenaphthylene [78536-16-0] 30, Sb2O3 20, and 2,6-di-tert-butylphenol 0.5 part mixed by a 120°-heat roller, 3 parts dicumyl peroxide [80-43-3] was added at 20-70°, and the mixture was hot-pressed at 160° for 30 min to form 1- or 3-mm-thick sheets. No bloom appeared on a sample kept in a 121° bath for 168 h and cooled to room temperature. Burning time (ASTM D 635-74) before and after the blooming test was unchanged at 4 s. The sample had O index 30% and residual fire-retardant (after Soxhlet extraction) 72%.

IC C08F291-00; C08F002-44; C08K005-03

CC 36-6 (Plastics Manufacture and Processing)

IT 78536-19-3 78536-20-6

RL: USES (Uses)

(fireproofing agents, for EPDM rubber)

IT 78536-18-2

RL: USES (Uses)

(fireproofing agents, for ethylene-vinyl acetate copolymer)

IT 78536-16-0 78536-17-1

RL: USES (Uses)

(fireproofing agents, for polyethylene)

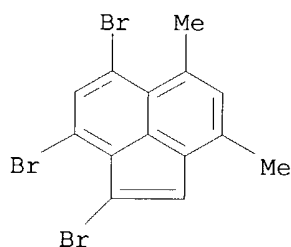
IT 78536-19-3

RL: USES (Uses)

(fireproofing agents, for EPDM rubber)

RN 78536-19-3 HCAPLUS

CN Acenaphthylene, 1,6,8-tribromo-3,5-dimethyl- (9CI) (CA INDEX NAME)



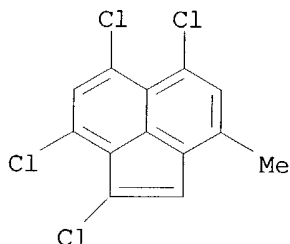
IT 78536-18-2

RL: USES (Uses)

(fireproofing agents, for ethylene-vinyl acetate copolymer)

RN 78536-18-2 HCAPLUS

CN Acenaphthylene, 1,5,6,8-tetrachloro-3-methyl- (9CI) (CA INDEX NAME)



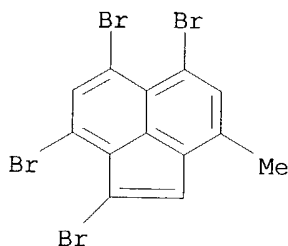
IT 78536-16-0

RL: USES (Uses)

(fireproofing agents, for polyethylene)

RN 78536-16-0 HCAPLUS

CN Acenaphthylene, 1,5,6,8-tetrabromo-3-methyl- (9CI) (CA INDEX NAME)



L53 ANSWER 27 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1981:31904 HCAPLUS

DN 94:31904

TI Polymers and rubbers with good resistance to radiochemical degradation

PA Japan Atomic Energy Research Institute, Japan

SO Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 55106228	A2	19800814	JP 1979-4803	19790122
	JP 61050490	B4	19861105		
PRAI	JP 1979-4803		19790122		

AB Thermoplastic polymers or rubbers containing radical initiators and >0.5 weight percent (based on polymers) acenaphthylene derivs. having 0-4 C1-4 alkyl substituents are heated and molded to give products having good resistance to radiochem. degradation. Thus, 60:40 ethylene-propene rubber 100, 2,2,4-trimethyl-1,2-dihydroquinoline 0.5, dicumyl peroxide 3, S 0.1, calcined clay 100, and 5,6-dimethylacenaphthylene (I) 10 parts were rolled at 100° and pressed 20 min at 180° to give I-grafted rubber composition having tensile strength 0.65 and 0.69 kg/mm² before and after γ -irradiation in air to 100 Mrad, resp., and elongation 670 and 580%, resp., compared with 0.65, 0.45, 680, and 140, resp., for a similar composition without I.

IC C08J003-00; C08F032-08; C08K005-01; C09K003-12

CC 38-7 (Elastomers, Including Natural Rubber)

IT **76149-90-1**

RL: USES (Uses)

(graft, with improved resistance to radiochem. degradation)

IT **76149-90-1**

RL: USES (Uses)

(graft, with improved resistance to radiochem. degradation)

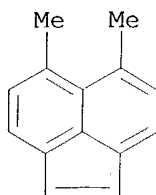
RN 76149-90-1 HCAPLUS

CN Acenaphthylene, 5,6-dimethyl-, polymer with ethene and 1-propene (9CI)
(CA INDEX NAME)

CM 1

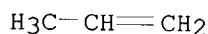
CRN 41002-83-9

CMF C14 H12



CM 2

CRN 115-07-1
CMF C3 H6



CM 3

CRN 74-85-1
CMF C2 H4



L53 ANSWER 28 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:508213 HCAPLUS

DN 85:108213

TI Electronic states of acenaphthylene. Linear dichroism in stretched polyethylene and magnetic circular dichroism

AU Thulstrup, Erik W.; Michl, Josef

CS Dep. Chem., Univ. Utah, Salt Lake City, UT, USA

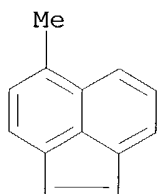
SO Journal of the American Chemical Society (1976), 98(15), 4533-40
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

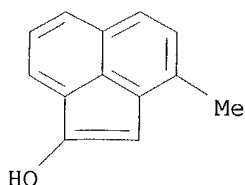
LA English

AB Low-temperature absorption, linear dichroic, and magnetic circular dichroic spectroscopy of acenaphthylene (I) and its 1,2-dibromo (II), 3-, 4-, and 5-fluoro, and 5-Me derivs. confirm previous assignments of five electronic states, detect a new one, and determine the directions of magnetic dipole transition moments between excited states; energies, intensities, polarizations, and signs of B terms agree with results of π -electron calcs. Systematic introduction of doubly excited configurations has little effect on the results for excited states assigned to the first five observed transitions; it suggests, however, that the newly observed excited state is predominantly doubly excited. The energy of the lowest triplet state of I was measured by the 0 perturbation technique. Measurement of polarized absorption in stretched polyethylene ("stretched-sheet method") yields the correct absolute polarizations even for a nearly circular mol. such as I; the expected reversal of preferred orientation on going to II is observed. The results demand a 2-parameter description of the orientation distribution and provide a good example for the inadequacy of 1-parameter

evaluation methods which are still occasionally used.
 CC 22-8 (Physical Organic Chemistry)
 IT 208-96-8 13019-33-5 17521-01-6 **19345-91-6** 20371-47-5
 21502-72-7
 RL: PRP (Properties)
 (electron configuration of, spectra in relation to)
 IT **19345-91-6**
 RL: PRP (Properties)
 (electron configuration of, spectra in relation to)
 RN 19345-91-6 HCAPLUS
 CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 29 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1976:104649 HCAPLUS
 DN 84:104649
 TI π, π -Biradicaloid hydrocarbons. The pleiadene family. II. A doubly excited state of pleiadene
 AU Kolc, Jaroslav; Downing, John W.; Manzara, Anthony P.; Michl, Josef
 CS Dep. Chem., Univ. Utah, Salt Lake City, UT, USA
 SO Journal of the American Chemical Society (1976), 98(4), 930-7
 CODEN: JACSAT; ISSN: 0002-7863
 DT Journal
 LA English
 AB Eleven excited singlet states in the uv spectra of pleiadene, five methylpleiadenes, and two dimethylpleiadenes were assigned for the absorptions between 200 and 1000 nm. Ti-electron calcns. (PPP-CI) account for the results and indicate that the second lowest excited state is doubly excited. The second transition involves promotion of both electrons from the highest occupied MO to the lowest unoccupied MO.
 CC 22-2 (Physical Organic Chemistry)
 IT **59012-07-6**
 RL: PRP (Properties)
 (3-methylacenaphthylene from)
 IT **19345-94-9P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with benzyne)
 IT **19345-91-6P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction with benzyne)
 IT **59012-07-6**
 RL: PRP (Properties)
 (3-methylacenaphthylene from)
 RN 59012-07-6 HCAPLUS
 CN 1-Acenaphthylenol, 3-methyl- (9CI) (CA INDEX NAME)

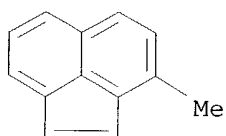


IT 19345-94-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with benzyne)

RN 19345-94-9 HCAPLUS

CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)

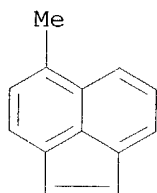


IT 19345-91-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with benzyne)

RN 19345-91-6 HCAPLUS

CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 30 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1976:74018 HCAPLUS

DN 84:74018

TI Application of the method for thiophene heterocycle synthesis using sodium sulfide to the preparation of sulfur analogs of polycyclic aromatic hydrocarbons

AU Cagniant, Paul; Kirsch, Gilbert

CS Fac. Sci., Univ. Metz, Metz, Fr.

SO Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1975), 281(11), 393-5

CODEN: CHDCAQ; ISSN: 0567-6541

DT Journal

LA French

OS CASREACT 84:74018

AB Naphtho[1,2-b]thiophene, thieno[3,2-g]benzothiophene, acenaphtho[1,2-b]thiophene, acenaphtho[4,5-b]thiophene, phenanthro[1,2-b]thiophene, phenanthro[4,3-b]thiophene, and acephenanthro[7,8-b]thiophene ring systems

were prepared by Vilsmeier-Haack formylation of tetrahydroarom. ketones, condensation of the chloroformyl derivs. with Na₂S-BrCH₂CRCO₂Et (R = H, Me), and aromatization with dichlorodicyanoquinone.

CC 27-9 (Heterocyclic Compounds (One Hetero Atom))

IT 3262-03-1P 49665-04-5P 58231-27-9P 58231-28-0P 58231-29-1P
58231-30-4P 58231-31-5P 58231-32-6P 58231-33-7P
 58231-34-8P

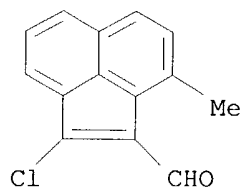
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with sodium sulfide and bromoalkanoate)

IT **58231-30-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with sodium sulfide and bromoalkanoate)

RN 58231-30-4 HCAPLUS

CN 1-Acenaphthylenecarboxaldehyde, 2-chloro-8-methyl- (9CI) (CA INDEX NAME)



L53 ANSWER 31 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1973:546892 HCAPLUS

DN 79:146892

TI Cationic polymerization of acenaphthylene and methylacenaphthylenes

AU Cohen, S.; Belliard, P.; Marechal, E.

CS Inst. Natl. Super. Chim. Ind. Rouen, Mont-Saint-Aignan, Fr.

SO Polymer (1973), 14(8), 352-4
 CODEN: POLMAG; ISSN: 0032-3861

DT Journal

LA English

AB The kinetics and reactivity ratio compared with PhCH:CH₂ were determined for the polymerization of acenaphthylenet(I) [208-96-8] initiated by stannic chloride [7646-78-8]. Comparison of exptl. with Hueckel MO and Pople complete neglect of differential overlap MO calcns. of stabilization energies indicated the contribution of ring strain to the reactivity of I. Reactivity ratios and stabilization energies were determined for the polymerization of 1-methylacenaphthylene [19345-99-4], 3-methylacenaphthylene [19345-94-9], and 5-methylacenaphthylene [19345-91-6].

CC 35-4 (Synthetic High Polymers)

IT **19345-91-6 19345-94-9** 19345-99-4

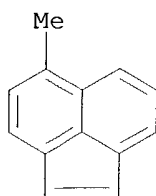
RL: RCT (Reactant); RACT (Reactant or reagent)
 (polymerization of, reactivity in)

IT **19345-91-6 19345-94-9**

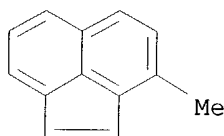
RL: RCT (Reactant); RACT (Reactant or reagent)
 (polymerization of, reactivity in)

RN 19345-91-6 HCAPLUS

CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)

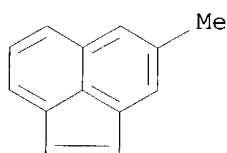


RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)

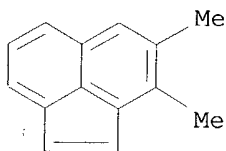


L53 ANSWER 32 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:72715 HCAPLUS
DN 78:72715
TI Cationic polymerization and copolymerization of methylacenaphthylenes
AU Belliard, Patrick; Marechal, Ernest
CS Lab. Chim. Macromol., Inst. Natl. Super. Chim. Ind., Rouen, Fr.
SO Bulletin de la Societe Chimique de France (1972), (11), 4255-75
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA French
AB High purity 1-methylacenaphthylene (I) [19345-99-4], 3-methylacenaphthylene [19345-94-9], and 5-methylacenaphthylene [19345-91-6] were prepared; steric hindrance in I prevented polymerization and copolymn., and only the lower oligomers were formed. Data for poly(3-methylacenaphthylene) [38723-82-9], poly(5-methylacenaphthylene) [38723-83-0], 3-methylacenaphthylene-styrene copolymer [38720-69-3], and 5-methylacenaphthylene-styrene copolymer [38720-70-6] agreed with CNDO II (J. A. Pople, 1965) calcns. rather than with Hueckel calcns. The effects of 5-C ring strain on acenaphthylene carbocation formation were discussed.
CC 35-4 (Synthetic High Polymers)
Section cross-reference(s): 26
IT 19345-97-2 41002-77-1 41002-78-2
41002-79-3 41002-80-6 41002-81-7
41002-82-8 41002-83-9 41002-84-0
41002-85-1 41002-86-2 41002-87-3
41002-88-4 41002-89-5 41002-90-8
41002-91-9 41002-92-0 41002-93-1
41002-94-2 41002-95-3 41002-96-4
41002-97-5 41002-98-6 41002-99-7
41003-00-3 41003-01-4 41003-02-5
41003-03-6 41003-04-7 41003-05-8
41082-61-5 41082-62-6 41237-23-4
RL: PRP (Properties)
(mol. orbitals of, calcn. of)
IT 85-08-5P 2435-82-7P 19345-91-6P 19345-94-9P
19345-99-4P 38723-82-9P 38723-83-0P 40908-02-9P
40908-03-0P 40908-04-1P 41002-74-8P

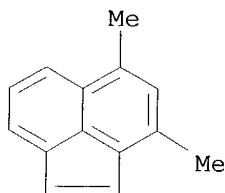
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 30347-44-5P **38720-69-3P 38720-70-6P** 40908-05-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, reactivity ratios in)
 IT **19345-97-2 41002-77-1 41002-78-2**
41002-79-3 41002-80-6 41002-81-7
41002-82-8 41002-83-9 41002-84-0
41002-85-1 41002-86-2 41002-87-3
41002-88-4 41002-89-5 41002-90-8
41002-91-9 41002-92-0 41002-93-1
41002-94-2 41002-95-3 41002-96-4
41002-97-5 41002-98-6 41002-99-7
41003-00-3 41003-01-4 41003-02-5
41003-03-6 41003-04-7 41003-05-8
41082-61-5 41082-62-6
 RL: PRP (Properties)
 (mol. orbitals of, calcn. of)
 RN 19345-97-2 HCAPLUS
 CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



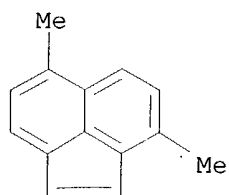
RN 41002-77-1 HCAPLUS
 CN Acenaphthylene, 3,4-dimethyl- (9CI) (CA INDEX NAME)



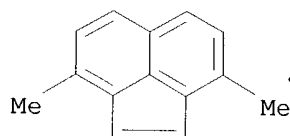
RN 41002-78-2 HCAPLUS
 CN Acenaphthylene, 3,5-dimethyl- (9CI) (CA INDEX NAME)



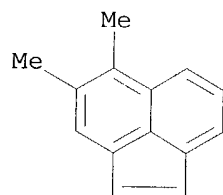
RN 41002-79-3 HCAPLUS
 CN Acenaphthylene, 3,6-dimethyl- (9CI) (CA INDEX NAME)



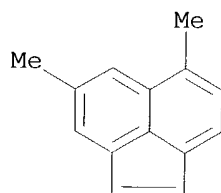
RN 41002-80-6 HCAPLUS
CN Acenaphthylene, 3,8-dimethyl- (6CI, 9CI) (CA INDEX NAME)



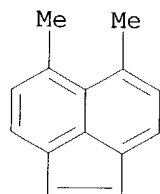
RN 41002-81-7 HCAPLUS
CN Acenaphthylene, 4,5-dimethyl- (9CI) (CA INDEX NAME)



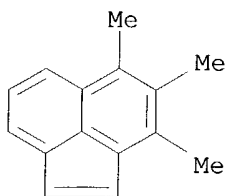
RN 41002-82-8 HCAPLUS
CN Acenaphthylene, 4,6-dimethyl- (9CI) (CA INDEX NAME)



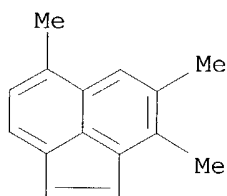
RN 41002-83-9 HCAPLUS
CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



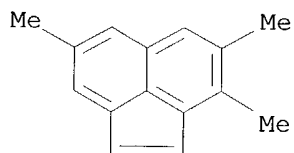
RN 41002-84-0 HCAPLUS
CN Acenaphthylene, 3,4,5-trimethyl- (9CI) (CA INDEX NAME)



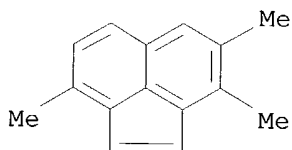
RN 41002-85-1 HCAPLUS
CN Acenaphthylene, 3,4,6-trimethyl- (9CI) (CA INDEX NAME)



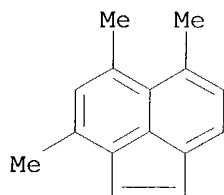
RN 41002-86-2 HCAPLUS
CN Acenaphthylene, 3,4,7-trimethyl- (9CI) (CA INDEX NAME)



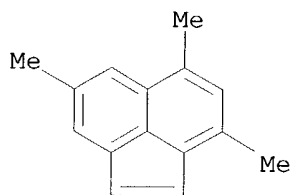
RN 41002-87-3 HCAPLUS
CN Acenaphthylene, 3,4,8-trimethyl- (9CI) (CA INDEX NAME)



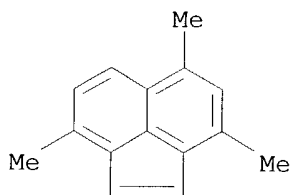
RN 41002-88-4 HCAPLUS
CN Acenaphthylene, 3,5,6-trimethyl- (9CI) (CA INDEX NAME)



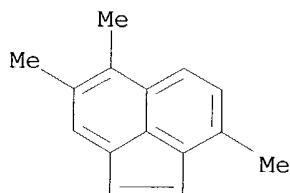
RN 41002-89-5 HCAPLUS
CN Acenaphthylene, 3,5,7-trimethyl- (9CI) (CA INDEX NAME)



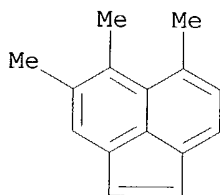
RN 41002-90-8 HCAPLUS
CN Acenaphthylene, 3,5,8-trimethyl- (9CI) (CA INDEX NAME)



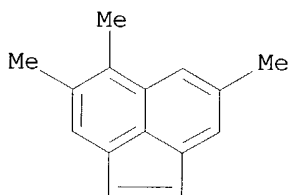
RN 41002-91-9 HCAPLUS
CN Acenaphthylene, 3,6,7-trimethyl- (9CI) (CA INDEX NAME)



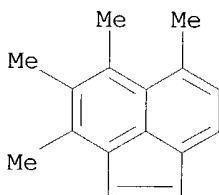
RN 41002-92-0 HCAPLUS
CN Acenaphthylene, 4,5,6-trimethyl- (9CI) (CA INDEX NAME)



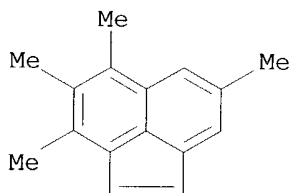
RN 41002-93-1 HCAPLUS
CN Acenaphthylene, 4,5,7-trimethyl- (9CI) (CA INDEX NAME)



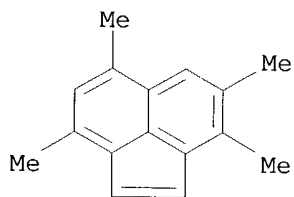
RN 41002-94-2 HCAPLUS
CN Acenaphthylene, 3,4,5,6-tetramethyl- (9CI) (CA INDEX NAME)



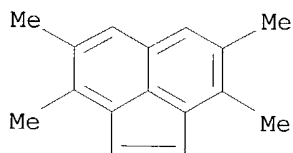
RN 41002-95-3 HCAPLUS
CN Acenaphthylene, 3,4,5,7-tetramethyl- (9CI) (CA INDEX NAME)



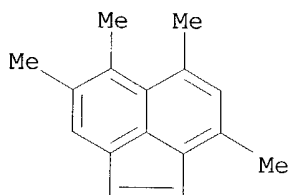
RN 41002-96-4 HCAPLUS
CN Acenaphthylene, 3,4,6,8-tetramethyl- (9CI) (CA INDEX NAME)



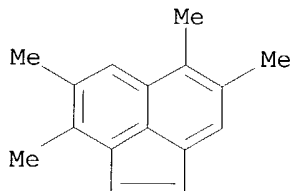
RN 41002-97-5 HCAPLUS
CN Acenaphthylene, 3,4,7,8-tetramethyl- (9CI) (CA INDEX NAME)



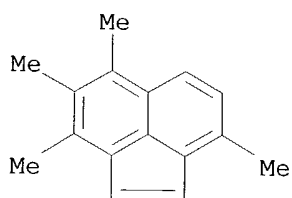
RN 41002-98-6 HCAPLUS
CN Acenaphthylene, 3,5,6,7-tetramethyl- (9CI) (CA INDEX NAME)



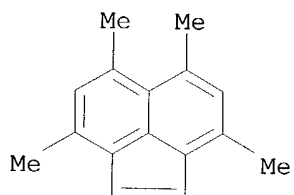
RN 41002-99-7 HCAPLUS
CN Acenaphthylene, 3,4,6,7-tetramethyl- (9CI) (CA INDEX NAME)



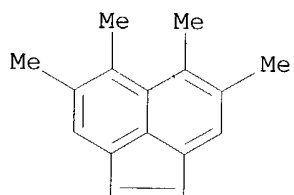
RN 41003-00-3 HCAPLUS
CN Acenaphthylene, 3,4,5,8-tetramethyl- (9CI) (CA INDEX NAME)



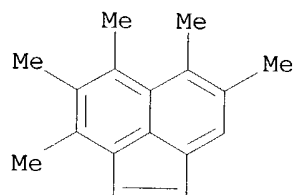
RN 41003-01-4 HCAPLUS
CN Acenaphthylene, 3,5,6,8-tetramethyl- (9CI) (CA INDEX NAME)



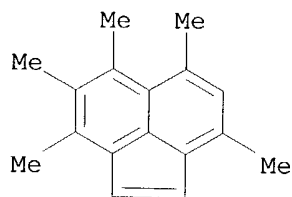
RN 41003-02-5 HCAPLUS
CN Acenaphthylene, 4,5,6,7-tetramethyl- (9CI) (CA INDEX NAME)



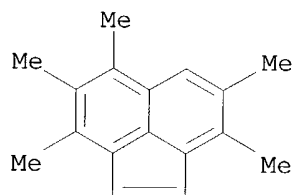
RN 41003-03-6 HCAPLUS
CN Acenaphthylene, 3,4,5,6,7-pentamethyl- (9CI) (CA INDEX NAME)



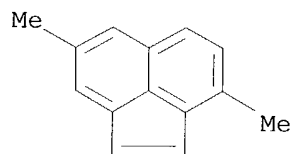
RN 41003-04-7 HCAPLUS
CN Acenaphthylene, 3,4,5,6,8-pentamethyl- (9CI) (CA INDEX NAME)



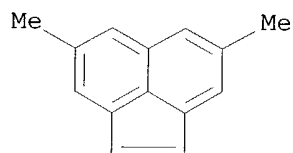
RN 41003-05-8 HCAPLUS
CN Acenaphthylene, 3,4,5,7,8-pentamethyl- (9CI) (CA INDEX NAME)



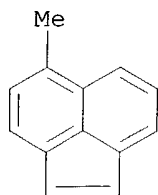
RN 41082-61-5 HCAPLUS
CN Acenaphthylene, 3,7-dimethyl- (9CI) (CA INDEX NAME)



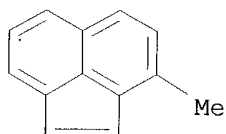
RN 41082-62-6 HCAPLUS
CN Acenaphthylene, 4,7-dimethyl- (9CI) (CA INDEX NAME)



IT **19345-91-6P 19345-94-9P 38723-82-9P**
38723-83-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19345-91-6 HCAPLUS
CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



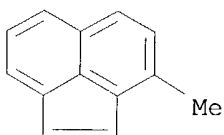
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 38723-82-9 HCAPLUS
CN Acenaphthylene, 3-methyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

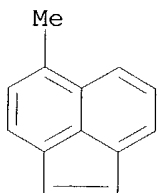
CRN 19345-94-9
CMF C13 H10



RN 38723-83-0 HCAPLUS
CN Acenaphthylene, 5-methyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 19345-91-6
CMF C13 H10



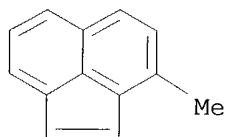
IT **38720-69-3P 38720-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, reactivity ratios in)
RN 38720-69-3 HCAPLUS

CN Acenaphthylene, 3-methyl-, polymer with ethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 19345-94-9

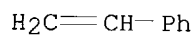
CMF C13 H10



CM 2

CRN 100-42-5

CMF C8 H8



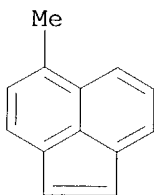
RN 38720-70-6 HCAPLUS

CN Acenaphthylene, 5-methyl-, polymer with ethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 19345-91-6

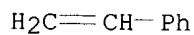
CMF C13 H10



CM 2

CRN 100-42-5

CMF C8 H8



L53 ANSWER 33 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1973:72624 HCAPLUS

DN 78:72624

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

TI Influence of the nature and position of substituents on the cationic polymerization of some aromatic monomers
 AU Marechal, E.
 CS Lab. Chim. Macromol., Inst. Natl. Super. Chim. Ind., Rouen, Fr.
 SO Journal of Macromolecular Science, Chemistry (1973), 7(2), 433-60
 CODEN: JMCHBD; ISSN: 0022-233X
 DT Journal
 LA English
 AB Studies of the cationic polymerization of methylated and methoxylated monomers
 by reactivity expts. and by quantum chemical theory indicated that although the results from the methods often agreed, discrepancies developed due to side phenomena. The phenomena included preliminary isomerization of the monomer, the ring strain effect, the effect of a substituent on monomer planarity, and complex formation.

CC 35-1 (Synthetic High Polymers)

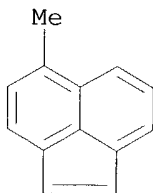
IT 95-15-8 100-42-5, reactions 100-80-1 208-96-8 232-54-2 232-55-3
 268-40-6 271-89-6 611-15-4 612-15-7 622-97-9 626-20-0 637-69-4
 707-96-0 769-25-5 787-61-1 2039-89-6 2039-90-9 2234-20-0
 3469-07-6 3469-08-7 3937-24-4 5379-20-4 6380-23-0 7530-35-0
 13400-02-7 14568-68-4 16657-08-2 17055-36-6 17598-03-7
19345-91-6 19345-94-9 19345-97-2 19345-99-4
 21897-50-7 22430-63-3 22484-28-2 23288-07-5 23288-08-6
 23288-09-7 23288-10-0 23288-11-1 24345-63-9 24387-09-5
 24407-19-0 27831-13-6 27973-23-5 28715-26-6 30566-10-0
 34985-47-2 35074-19-2 35074-20-5 39240-15-8 40243-62-7
 40243-64-9 40243-65-0 40243-66-1 40243-67-2 40243-68-3
 40243-69-4 40243-70-7 40243-71-8 40243-72-9 40243-73-0
 40243-74-1 40243-75-2 40243-78-5 40243-79-6 40243-84-3
 40243-87-6 40243-89-8 40243-90-1 40243-91-2 40269-87-2

RL: RCT (Reactant); RACT (Reactant or reagent)
 (polymerization of, quantum chemical in relation to cationic)

IT **19345-91-6 19345-94-9 19345-97-2**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (polymerization of, quantum chemical in relation to cationic)

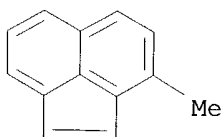
RN 19345-91-6 HCAPLUS

CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)

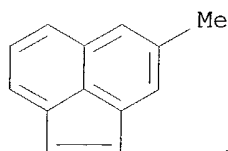


RN 19345-94-9 HCAPLUS

CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-97-2 HCAPLUS
 CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



L53 ANSWER 34 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1972:405179 HCAPLUS

DN 77:5179

TI 3- and 4-Formylpentane mixtures

IN Himmele, Walter; Aquila, Werner

PA Badische Anilin- & Soda-Fabrik AG

SO Ger. Offen., 8 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2051319	A	19720427	DE 1970-2051319	19701020
PRAI	DE 1970-2051319		19701020		

AB Five mixts. of $RR1CHCH2CH2CHO$ (I) and $RR1CHCH2CH2CHMeCHO$ [II; R = Ph or o-MeC₆H₄; R₁ = H, Me, Ph, or PhCH₂, or $RR1CH = 1,2,3,4$ -tetrahydro-1-naphthyl or acenaphthenyl], useful as perfumes, were prepared by hydroformylation of $RR1CHCH2CH:CHMe$ (III) in the presence of dimeric cyclooctadienylrhodium chloride (IV) at 100°/700 atm gage and the aldehydes formed optionally hydrogenated and acetylated. Thus, III (R = o-MeC₆H₄, R₁ = H) 176, C₆H₆300, and IV 0.05 part were heated 6 hr at 100°/700 atmospheric gage 1:1 CO-H pressure to give 177 parts mixture of I (R = o-MeC₆H₄, R₁ = H) and II (R = o-MeC₆H₄, R₁ = H) of flowery odor. The mixture (168 parts) was hydrogenated 12 hr over Raney Ni in MeOH at 80°/50 atmospheric to give 121 parts mixture of o-MeC₆H₄-(CH₂)₃CHMeCH₂OH and o-MeC₆H₄CH₂CH₂CH₂CH₂OH, which was refluxed 1 hr with Ac₂O to give a mixture of the acetates.

IC C07C

CC 25-15 (Noncondensed Aromatic Compounds)

Section cross-reference(s): 26, 62

IT 6047-69-4 36613-03-3 **36613-06-6** 36666-03-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydroformylation of, catalysts for)

IT 33856-83-6P 36612-96-1P 36612-97-2P 36612-98-3P 36612-99-4P

36613-01-1P 36613-02-2P 36613-04-4P 36613-05-5P **36613-07-7P**

36613-08-8P 36613-11-3P 36613-13-5P 36613-14-6P

36613-15-7P 36613-16-8P 36613-17-9P 36613-18-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

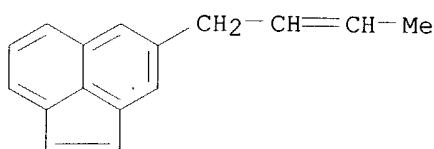
IT **36613-06-6**

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydroformylation of, catalysts for)

RN 36613-06-6 HCAPLUS

CN Acenaphthylene, 4-(2-butenyl)- (9CI) (CA INDEX NAME)

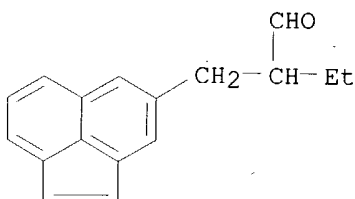


IT 36613-07-7P 36613-08-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

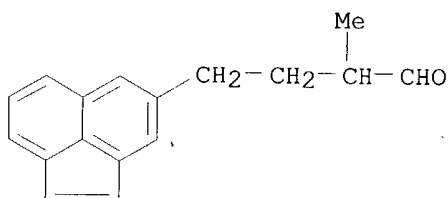
RN 36613-07-7 HCAPLUS

CN 4-Acenaphthylenepropanal, α -ethyl- (9CI) (CA INDEX NAME)



RN 36613-08-8 HCAPLUS

CN 4-Acenaphthylenebutanal, α -methyl- (9CI) (CA INDEX NAME)



L53 ANSWER 35 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1968:458969 HCAPLUS

DN 69:58969

TI Constituents of cigaret smoke. XI. The isolation and synthesis of acenaphthylenes and macrocyclic polyolefins

AU Entwistle, I. D.; Johnstone, R. A. W.

CS Univ. Liverpool, Liverpool, UK

SO Journal of the Chemical Society [Section] C: Organic (1968), (14), 1818-22

CODEN: JSOOAX; ISSN: 0022-4952

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB Acenaphthylene, the monomethylacenaphthylenes, such as I, and some dimethylacenaphthylenes were identified in cigarette smoke condensate. Some of the acenaphthylenes were synthesized, as was also a perhydromacrocyclic compound (II). The possible formation of aromatic compounds from macrocyclic polyolefins is discussed, and the isolation of such a macrocycle from cigarette smoke is described. The mass spectra of some acenaphthylenes are described.

CC 26 (Condensed Aromatic Compounds)

IT 1786-12-5P 19335-98-9P 19345-88-1P 19345-89-2P 19345-90-5P
 19345-91-6P 19345-92-7P 19345-93-8P
 19345-94-9P 19345-95-0P 19345-96-1P
 19345-97-2P 19345-98-3P 19345-99-4P
 19346-00-0P 19346-01-1P 19346-02-2P
 19346-03-3P 19346-04-4P 19346-05-5P 19346-06-6P
 19346-07-7P 19346-08-8P 19346-09-9P 19346-10-2P 19565-21-0P
 20526-63-0P

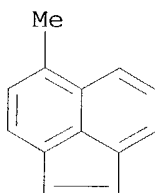
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 19345-91-6P 19345-92-7P 19345-94-9P
 19345-95-0P 19345-97-2P 19345-98-3P
 19346-00-0P 19346-01-1P 19346-02-2P
 19346-03-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 19345-91-6 HCAPLUS

CN Acenaphthylene, 5-methyl- (8CI, 9CI) (CA INDEX NAME)



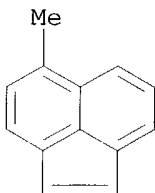
RN 19345-92-7 HCAPLUS

CN Acenaphthylene, 5-methyl-, compd. with 1,3,5-trinitrobenzene (1:1) (8CI)
 (CA INDEX NAME)

CM 1

CRN 19345-91-6

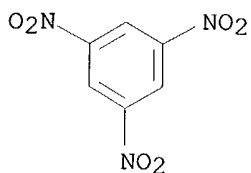
CMF C13 H10



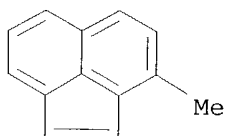
CM 2

CRN 99-35-4

CMF C6 H3 N3 O6



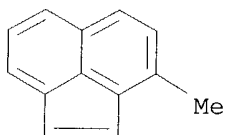
RN 19345-94-9 HCAPLUS
CN Acenaphthylene, 3-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-95-0 HCAPLUS
CN Acenaphthylene, 3-methyl-, compd. with 1,3,5-trinitrobenzene (1:1) (8CI)
(CA INDEX NAME)

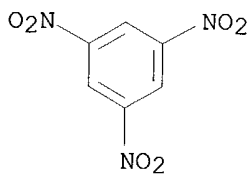
CM 1

CRN 19345-94-9
CMF C13 H10

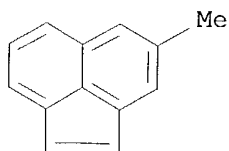


CM 2

CRN 99-35-4
CMF C6 H3 N3 O6



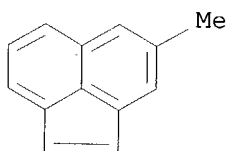
RN 19345-97-2 HCAPLUS
CN Acenaphthylene, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 19345-98-3 HCAPLUS
CN Acenaphthylene, 4-methyl-, compd. with 1,3,5-trinitrobenzene (1:1) (8CI)
(CA INDEX NAME)

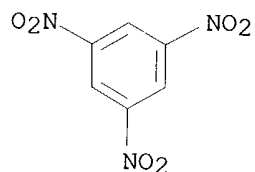
CM 1

CRN 19345-97-2
CMF C13 H10

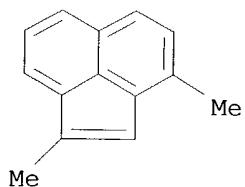


CM 2

CRN 99-35-4
CMF C6 H3 N3 O6



RN 19346-00-0 HCAPLUS
CN Acenaphthylene, 1,3-dimethyl- (8CI) (CA INDEX NAME)

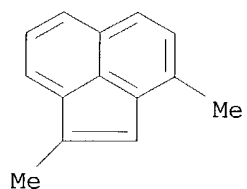


RN 19346-01-1 HCAPLUS
CN Acenaphthylene, 1,3-dimethyl-, compd. with 1,3,5-trinitrobenzene (1:1)
(8CI) (CA INDEX NAME)

CM 1

CRN 19346-00-0

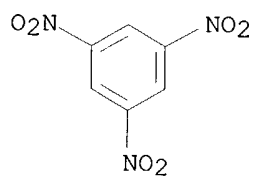
CMF C14 H12



CM 2

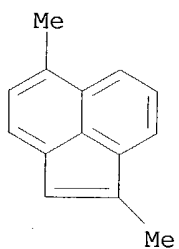
CRN 99-35-4

CMF C6 H3 N3 O6



RN 19346-02-2 HCAPLUS

CN Acenaphthylene, 1,5-dimethyl- (8CI) (CA INDEX NAME)



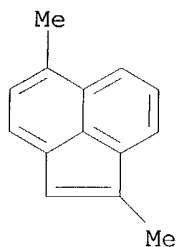
RN 19346-03-3 HCAPLUS

CN Acenaphthylene, 1,5-dimethyl-, compd. with 1,3,5-trinitrobenzene (1:1)
(8CI) (CA INDEX NAME)

CM 1

CRN 19346-02-2

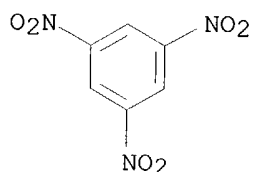
CMF C14 H12



CM 2

CRN 99-35-4

CMF C6 H3 N3 O6



- L53 ANSWER 36 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1968:16234 HCAPLUS
 DN 68:16234
 TI Tables of quantum chemical data. XIV. Energy characteristics of some hydrocarbons with exocyclic methylene group
 AU Tichy, Milos; Zahradnik, Rudolf
 CS Ustav Hyg. Prace Chorob Povolani, Prague, Czech.
 SO Collection of Czechoslovak Chemical Communications (1967), 32(12), 4485-91
 CODEN: CCCCAK; ISSN: 0010-0765
 DT Journal
 LA English
 AB Hueckel energy characteristics of derivs. formed by attaching a 2pz atomic orbital to an even alternant, odd alternant, or nonalternant hydrocarbon system were tabulated. Included are: nos. of π -electrons and of C-C σ -bonds, total π -electronic energy, sp. delocalization energy, energies of the 2 highest occupied and of the 2 lowest unoccupied M.O., and energy of the $N \rightarrow V1$ transition.
 CC 65 (General Physical Chemistry)
 IT 497-20-1 539-79-7 4095-06-1 12341-14-9, Pentalene, 1,?-dihydro-1-methylene-, ion(1-) 12341-15-0, Pentalenylium, 2,?-dihydro-2-methylene- 12341-29-6, Azulenylium, 2,?-dihydro-2-methylene- 12341-30-9, Azulenylium, 1,?-dihydro-1-methylene- 12341-31-0, Azulene, 4,?-dihydro-4-methylene-, ion(1-) 12341-32-1, Azulenylium, 5,?-dihydro-5-methylene- 12341-33-2, Azulene, 6,?-dihydro-6-methylene-, ion(1-) 12341-56-9, Cyclohexadienylium, 6-methylene-3-phenyl- 12341-57-0, Heptalenylium, 1,?-dihydro-1-methylene- 12341-58-1, Heptalenylium, 2,?-dihydro-2-methylene- 12341-59-2, Heptalenylium, 3,?-dihydro-3-methylene- 12341-60-5, Acenaphthylenylium, 1,?-dihydro-1-methylene- **12341-61-6**, Acenaphthylene, 3,?-dihydro-3-methylene, ion(1-) 12341-62-7, Acenaphthylenylium, 4,?-dihydro-4-methylene- 12341-77-4, Anthracenylium,

1,?-dihydro-1-methylene- 12341-78-5, Anthracenylium,
 2,?-dihydro-2-methylene- 12341-79-6, Anthracenylium,
 9,?-dihydro-9-methylene- 12341-80-9, Phenanthrenylium,
 4,?-dihydro-4-methylene- 12341-81-0, Phenanthrenylium,
 3,?-dihydro-3-methylene- 12341-82-1, Phenanthrenylium,
 2,?-dihydro-2-methylene- 12341-83-2, Phenanthrenylium,
 1,?-dihydro-1-methylene- 12341-84-3, Phenanthrenylium,
 9,?-dihydro-9-methylene- 12342-02-8, Fluoranthene, 3,?-dihydro-3-
 methylene-, ion(1-) 12342-03-9, Fluoranthene, 1,?-dihydro-1-methylene-,
 ion(1-) 12342-04-0, Fluoranthenylium, 2,?-dihydro-2-methylene-
 12342-05-1, Fluoranthenylium, 7,?-dihydro-7-methylene- 12342-06-2,
 Fluoranthenylium, 8,?-dihydro-8-methylene- 12342-07-3,
 Acephenanthrylenylium, 2,?-dihydro-2-methylene- 12342-08-4,
 Acephenanthrylenylium, 10,?-dihydro-10-methylene- 12342-09-5,
 Acephenanthrylenylium, 8,?-dihydro-8-methylene- 12342-10-8,
 Acephenanthrylenylium, 5,?-dihydro-5-methylene- 12342-11-9,
 Acephenanthrylenylium, 4,?-dihydro-4-methylene- 12342-12-0,
 Aceanthrylenylium, 4,?-dihydro-4-methylene- 12342-13-1,
 Aceanthrylenylium, 8,?-dihydro-8-methylene- 12342-14-2, Pyrenylium,
 2,?-dihydro-2-methylene- 12342-15-3, Aceanthrylenylium,
 10,?-dihydro-10-methylene- 12342-16-4, Pyrenylium, 1,?-dihydro-1-
 methylene- 12342-17-5, Pyrenylium, 4,?-dihydro-4-methylene-
 12342-18-6, Aceanthrylenylium, 2,?-dihydro-2-methylene- 12342-19-7,
 Aceanthrylenylium, 1,?-dihydro-1-methylene- 12342-29-9, Naphthacenylium,
 5,?-dihydro-5-methylene- 12342-30-2, Naphthacenylium,
 1,?-dihydro-1-methylene- 12342-31-3, Naphthacenylium,
 2,?-dihydro-2-methylene- 12342-32-4, Benz[a]anthracenylium,
 1,?-dihydro-1-methylene- 12342-33-5, Benz[a]anthracenylium,
 2,?-dihydro-2-methylene- 12342-34-6, Benz[a]anthracenylium,
 3,?-dihydro-3-methylene- 12342-35-7, Benz[a]anthracenylium,
 4,?-dihydro-4-methylene- 12342-36-8, Benz[a]anthracenylium,
 5,?-dihydro-5-methylene- 12342-37-9, Benz[a]anthracenylium,
 6,?-dihydro-6-methylene- 12342-38-0, Benz[a]anthracenylium,
 7,?-dihydro-7-methylene- 12342-39-1, Benz[a]anthracenylium,
 8,?-dihydro-8-methylene- 12342-40-4, Benz[a]anthracenylium,
 9,?-dihydro-9-methylene- 12342-41-5, Benz[a]anthracenylium,
 10,?-dihydro-10-methylene- 12342-42-6, Benz[a]anthracenylium,
 11,?-dihydro-11-methylene- 12342-43-7, Benz[a]anthracenylium,
 12,?-dihydro-12-methylene- 12342-44-8, Triphenylenylium,
 2,?-dihydro-2-methylene- 12342-45-9, Triphenylenylium,
 1,?-dihydro-1-methylene- 12342-46-0, Chrysenylium, 5,?-dihydro-5-
 methylene- 12342-47-1, Chrysenylium, 6,?-dihydro-6-methylene-
 12342-48-2, Chrysenylium, 1,?-dihydro-1-methylene- 12342-49-3,
 Chrysenylium, 2,?-dihydro-2-methylene- 12342-50-6, Chrysenylium,
 3,?-dihydro-3-methylene- 12342-51-7, Chrysenylium, 4,?-dihydro-4-
 methylene- 12342-52-8, Benzo[c]phenanthrenylium, 1,?-dihydro-1-methylene-
 12342-53-9, Benzo[c]phenanthrenylium, 2,?-dihydro-2-methylene-
 12342-54-0, Benzo[c]phenanthrenylium, 3,?-dihydro-3-methylene-
 12342-55-1, Benzo[c]phenanthrenylium, 4,?-dihydro-4-methylene-
 12342-56-2, Benzo[c]phenanthrenylium, 5,?-dihydro-5-methylene-
 12342-57-3, Benzo[c]phenanthrenylium, 6,?-dihydro-6-methylene-
 12342-65-3, Benzo[k]fluoranthene, 3,?-dihydro-3-methylene-, ion(1-)
 12342-74-4, Benz[a]aceanthrylenylium, 4,?-dihydro-4-methylene-
 12342-75-5, Benz[a]aceanthrylenylium, 3,?-dihydro-3-methylene-
 12342-76-6, Benz[a]aceanthrylenylium, 2,?-dihydro-2-methylene-
 12342-77-7, Benz[a]aceanthrylenylium, 1,?-dihydro-1-methylene-
 12342-78-8, Benz[a]aceanthrylenylium, 12,?-dihydro-12-methylene-
 12342-79-9, Benz[a]aceanthrylenylium, 10,?-dihydro-10-methylene-
 12342-80-2, Benz[a]aceanthrylenylium, 6,?-dihydro-6-methylene-

12342-81-3, Cyclopenta[fg]naphthacenylium, 1,?-dihydro-1-methylene-
 12342-82-4, Cyclopenta[fg]naphthacenylium, 3,?-dihydro-3-methylene-
 12342-83-5, Cyclopenta[fg]naphthacenylium, 5,?-dihydro-5-methylene-
 13538-66-4 13538-67-5 19463-03-7 19463-04-8 19463-05-9
 19463-06-0 19463-07-1 19463-08-2 19463-09-3 19463-10-6
 19463-11-7 19463-12-8 19463-13-9 19463-14-0 19463-15-1
 19463-16-2 19463-17-3 19463-18-4 19463-19-5 19463-20-8
 19463-21-9 19463-22-0 19463-23-1 19463-24-2 19463-25-3
 19463-26-4 19463-27-5 19463-28-6 19463-29-7 19463-30-0
 19463-31-1 19463-32-2 19463-33-3 19463-34-4 19463-35-5
 19463-36-6 19463-37-7 19463-38-8 20184-16-1

RL: PRP (Properties)

(energy levels of, calcn. of)

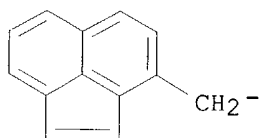
IT 12341-61-6, Acenaphthylene, 3,?-dihydro-3-methylene, ion(1-)

RL: PRP (Properties)

(energy levels of, calcn. of)

RN 12341-61-6 HCAPLUS

CN Acenaphthylene, 3,?-dihydro-3-methylene-, ion(1-) (9CI) (CA INDEX NAME)



L53 ANSWER 37 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1966:35691 HCAPLUS

DN 64:35691

OREF 64:6588b-h, 6589a-c

TI Pleiadene systems. II. Mechanism of acepleiadylene formation; a vinologous elimination in the acenaphthene series

AU Cava, M. P.; Merkel, K. E.; Schlessinger, R. H.

CS Ohio State Univ., Columbus

SO Tetrahedron (1965), 21(11), 3059-64

CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB cf. preceding abstract The conversion of 5,10-dihydroacepleiadene-5,10-diol (I) into acepleiadylene (II) by brief treatment with acid or by warming with p-MeC6H4SO2Cl in C5H5N appeared to involve 2 consecutive vinylogous eliminations. It was anticipated that the simpler model compound, 5-(α -hydroxybenzyl)acenaphthene (III) would similarly undergo vinylogous dehydration to the p-quinodimethane (IV), whose prototropic rearrangement would give the fully aromatic 5-benzylacenaphthylene (V). Acenaphthene (5.0 g.) and 3.7 ml. BzCl in 75 ml. C6H6 treated in 15 min. at 20° with 4.2 g. powdered AlCl3 and the mixture stirred 1 hr., poured into 100 ml. dilute HCl and extracted with Et2O, the isolated brown oil chromatographed on 100 g. neutral Al2O3 (Woelm, grade I) and eluted with C6H6 yielded 49% 5-benzoylacenaphthene (VI), m. 100-2°. VI (1.21 g.) and 0.5 g. NaBH4 in 70 ml. 4:3 C6H6-MeOH stirred 4 hrs. at 20° and the gelatinous residue on evaporation triturated with 10% aqueous NaOH yielded

95% III, m. 113-14° (C6H12). I (0.1 g.) and 0.1 g. p-MeC6H4SO2Cl in 20 ml. C5H5N refluxed (N atmospheric) 20 hrs. and the oily residue on evaporation

purified by chromatography over 20 g. neutral Al₂O₃ (Woelm, grade I), eluted with C₆H₁₂ and crystallized from C₆H₁₂ gave 58% V, m. 58°, τ 5.54, 2.95 (CDC13); N.M.R. spectrum of acenaphthylene, τ 2.92 (CDC13). V (0.1 g.) in 50 ml. alc. hydrogenated over 0.12 g. 5% Pd-C 1 hr. and the filtered (Celite) solution evaporated in vacuo yielded 99% 5-benzylacenaphthene (VII), m. 111°. By use of a Soxhlet extractor, 0.4 g. VI was introduced into 300 ml. Et₂O containing 0.65 g. LiAlH₄ and 6.3 g. AlCl₃ in 2 hrs., the mixture decomposed with 100 ml. H₂O and extracted with 200 ml. Et₂O

to

yield 93% VII, m. 111°, identical with the material obtained by reduction of VI. It was thus demonstrated that III could be converted to V by dehydration with p-MeC₆H₄SO₂Cl in C₅H₅N. The analogous dehydration of 4-(α -hydroxybenzyl)acenaphthene (VIII) to 4-benzylacenaphthylene (IX) by way of a quinoid intermediate should not occur unless a hydride transfer mechanism involving carbonium ions were operative which would also be valid for conversion of III to V. An improved procedure for the synthesis of VIII was developed. Acenaphthene (100 g.) in 800 ml. AcOH stirred rapidly with addition of 125 ml. 70% aqueous HNO₃ in 15 min. and the cooled mixture diluted to 2 l. with H₂O yielded 87% 5-nitroacenaphthene, m. 104°. The nitro compound (50.0 g.), 2.5 g. 10% Pd-C, and 60 ml. 85% N₂H₄.H₂O refluxed 45 min. in 1.0 l. 95% alc. and the hot filtered solution (Celite) diluted with H₂O yielded 95% 5-aminoacenaphthene, m. 104°, acetylated with Ac₂O-C₅H₅N to yield 95% 5-acetamidoacenaphthene, m. 190°. The amide (10.0 g.) in 900 ml. AcOH treated for 15 min. with 70 ml. 70% aqueous HNO₃ and the mixture stirred 30 min., diluted with 2.0 l.

H₂O

and the product refluxed 24 hrs. in 600 ml. alc. and 80 ml. 70% aqueous H₂SO₄, the hydrolysis mixture evaporated to approx. 225 ml. and cooled to 10° gave 3.94 g. of dark red needles of 4-nitro-5-aminoacenaphthene (X), m. 235°. X (11.0 g.) in 150 ml. AcOH and 15 ml. concentrated H₂SO₄ added to 6.0 g. NaNO₂ in 50 ml. concentrated H₂SO₄ at 0-20° and the mixture kept 1 hr. at 20°, the diazonium solution added slowly to a mixture of 14.0 g. CuSO₄.5H₂O, 180 ml. H₃PO₂, and 100 ml. 95% alc. and kept 1 hr. before dilution with 1.5 l. ice-H₂O, extracted with 300 ml. EtOAc, and the isolated product chromatographed over 60 g. neutral Al₂O₃ (Woelm, grade II), eluted with C₆H₆, and crystallized from C₆H₆ gave 60% yield of 4-nitroacenaphthene, m. 130-2°. The nitro compound (20.0 g.) in 1.0 l. alc. containing 30 ml. 85% N₂H₄.H₂O refluxed 2 hrs. with 2.0 g. 10% Pd-C and the filtered solution (Celite) evaporated to 100 ml., diluted with H₂O to complete crystallization,

and

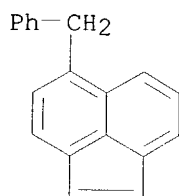
filtered gave 16.4 g. needles of 4-aminoacenaphthene, m. 88-9°. The amino compound (10.0 g.) in 25 ml. concentrated aqueous HCl and 115 ml. H₂O diazotized at 0° with 4.5 g. NaNO₂ in 50 ml. H₂O, and the mixture stirred 1 hr., treated with 10.0 g. Hg(NO₃)₂ and 15.0 g. NaBr in 50 ml. H₂O and the air-dried complex decomposed at 100° in 30 min. in the presence of 50.0 g. powdered NaBr, the decomposition residue extracted with C₆H₆, and

the product purified from C₆H₆ by chromatography over 40 g. neutral Al₂O₃ gave a yellow solid, sublimed to yield 37% 4-bromoacenaphthene, m. 65-6°. The bromo compound (5.199 g.) and 3.6 g. CuCN refluxed 4 hrs. in 25 ml. freshly distilled N-methylpyrrolidone and the mixture poured into 15 ml. H₂O and 4 ml. concentrated HCl containing 10.0 g. FeCl₃, the mixture heated 20

min. on a steam bath and extracted with CHCl₃, the isolated oily product chromatographed over 40 g. neutral Al₂O₃ (Woelm, grade I) and eluted with C₆H₆ yielded 71% 4-cyanoacenaphthene, m. 106-7°. The cyano derivative (0.105 g.) in 40 ml. Et₂O stirred 4 hrs. at 20° with 3.0 ml. 3M ethereal PhMgBr and the mixture poured into 15 ml. concentrated aqueous HCl, filtered,

and the yellow imine HCl salt boiled in alc., the hydrolysis mixture diluted with 200 ml. CHCl₃ and filtered from precipitated NH₄Cl, the filtrate evaporated and the residue crystallized from alc. gave an 82% yield of 4-benzoylacenaphthene, m. 97.0-8.5°. The ketone (1.0 g.) stirred 4 hrs. in 125 ml. Et₂O with 1.0 g. LiAlH₄ at 20° and the mixture diluted with 100 ml. H₂O, the product isolated, and the white solid (0.88 g.) crystallized from C₆H₁₄ gave 88% yield of VIII, m. 86-7°. VIII (0.1 g.) and 0.15 g. p-MeC₆H₄SO₂Cl in 20 ml. C₅H₅N refluxed (N atmospheric) 24 hrs. yielded only unchanged VIII.

CC 36 (Condensed Aromatic Compounds)
 IT 4624-38-8, Acenaphthylene, 5-benzyl-
 (formation from α -phenyl-5-acenaphthenemethanol)
 IT 4624-38-8, Acenaphthylene, 5-benzyl-
 (formation from α -phenyl-5-acenaphthenemethanol)
 RN 4624-38-8 HCAPLUS
 CN Acenaphthylene, 5-benzyl- (7CI, 8CI) (CA INDEX NAME)



L53 ANSWER 38 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1964:476383 HCAPLUS

DN 61:76383

OREF 61:13253g-h,13254a-d

TI Alkaline degradation of 1,1-disubstituted sulfonylhydrazides. Synthesis of a pair of cyclic, benzylic hydrazines derived from acenaphthene and acenaphthylene

AU Carpino, Louis A.; Goewicke, Siegfried

CS Univ. of Massachusetts, Amherst

SO Journal of Organic Chemistry (1964), 29(10), 2824-30

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

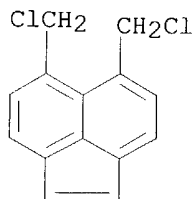
GI For diagram(s), see printed CA Issue.

AB In order to test some hypotheses relating to the oxidation and sulfonylhydrazide degradation of 1,1-disubstituted hydrazines, 2 appropriate model hydrazines have been prepared for further study, namely 2-amino-2,3-dihydro-1H-indeno[1,6,7-def]isoquinoline (I) and 2-amino-2,3,6,7-tetrahydro-1H-indeno[1,6,7-def]isoquinoline (II). Treatment of acenaphthene-5,6-dicarboxylic acid anhydride with N₂H₄.H₂O gave the corresponding cyclic hydrazide (III), which was reduced by means of NaBH₄ and LiBr to II. An alternate route to II involved LiAlH₄ reduction of di-Me acenaphthene-5,6-dicarboxylate (IV) to the diol. Treatment of the diol with HBr gave the dibromide which upon treatment with tert-Bu carbazate and Et₃N in HCONMe₂ gave the carbo-tert-butoxy derivative (V) which was converted to II by cleavage with HCl. The most direct route to I involved treatment of 5,6-bis(bromomethyl)acenaphthene with N-bromosuccinimide to give the corresponding tribromide (VI). Treatment of VI with tert-Bu carbazate and Et₃N in HCONMe₂ was accompanied by dehydrobromination to give the protected, unsatd. hydrazine derivative (VII),

which on removal of the carbo-tert-butoxy group gave I. An alternate route to I involved bromination of IV with N-bromosuccinimide followed by dehydrobromination with LiBr in HCONMe₂ to the unsatd. diester (VIII), reduction of which by means of LiAlH₄ gave the unsatd. diol (IX). IX was converted to the dichloride by reaction with SOCl₂ in C₆H₆ and the dichloride was cyclized to VII by reaction with tert-Bu carbazate and Et₃N in HCONMe₂. The ultraviolet and nuclear magnetic resonance spectra of the substituted acenaphthene and acenaphthylene derivs. obtained during the course of this work were examined and correlated with the spectra of the parent hydrocarbons.

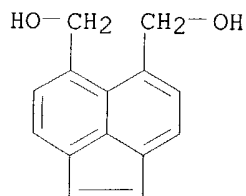
CC 36 (Condensed Aromatic Compounds)

IT 4599-95-5, Acenaphthene, 5,6-bis(bromomethyl)- 4599-96-6,
5,6-Acenaphthenedicarboxylic acid, dimethyl ester 4599-97-7,
5,6-Acenaphthenedimethanol 5699-00-3, 5,6-Acenaphthenedicarboxylic
anhydride 5699-11-6, 5,6-Acenaphthenedicarboximide, N-amino-
33758-39-3, Carbaniloyl chloride, N-ethyl- 92152-70-0, Acenaphthene,
1-bromo-5,6-bis(bromomethyl)- **92152-76-6**, Acenaphthylene,
5,6-bis(chloromethyl)- **92254-00-7**, 5,6-Acenaphthylenedimethanol
92853-25-3, 5,6-Acenaphthenedicarboxylic acid, 1,2-dibromo-, dimethyl
ester 92873-11-5, 5,6-Acenaphthenedicarboxylic acid, 1-bromo-, dimethyl
ester 92964-95-9, 5,6-Acenaphthylenedicarboxylic acid, dimethyl ester
94873-12-8, 5,6-Acenaphthenedicarboximide, N-(benzylideneamino)-
95515-99-4, 1H-Indeno[6,7,1-def]isoquinoline, 2-amino-2,3,6,7-tetrahydro-,
hydrochloride 98904-03-1, 2H-Indeno[6,7,1-def]isoquinoline-2-carbamic
acid, 1,3,6,7-tetrahydro-, tert-butyl ester 100259-57-2,
1H-Indeno[6,7,1-def]isoquinoline, 2-(benzylideneamino)-2,3,6,7-tetrahydro-
106194-80-3, p-Toluenesulfonamide, N-(1,3,6,7-tetrahydro-2H-indeno[6,7,1-
def]isoquinolin-2-yl)- 107101-72-4, 2H-Indeno[6,7,1-def]isoquinoline-2-
carbamic acid, 1,3-dihydro-, tert-butyl ester
(preparation of)
IT **92152-76-6**, Acenaphthylene, 5,6-bis(chloromethyl)-
92254-00-7, 5,6-Acenaphthylenedimethanol
(preparation of)
RN 92152-76-6 HCAPLUS
CN Acenaphthylene, 5,6-bis(chloromethyl)- (7CI) (CA INDEX NAME)



RN 92254-00-7 HCAPLUS

CN 5,6-Acenaphthylenedimethanol (7CI) (CA INDEX NAME)



L53 ANSWER 39 OF 39 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1961:124707 HCAPLUS
 DN 55:124707
 OREF 55:23456c-i,23457a-i,23458a-i,23459a-g
 TI Polymerization of acenaphthylene induced by tritylsodium and halted by
 "at-complexes." IV
 AU Wittig, Georg; Reppe, Hans G.; Eicher, Theophil
 CS Univ. Tübingen, Germany
 SO Ann. (1961), 643, 47-67
 DT Journal
 LA Unavailable
 OS CASREACT 55:124707
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 52, 1969g. (The term "at-complexes" signifies complexes formed by
 addition of an anion to a Lewis acid). $\text{Ph}_3\text{CNa(I)}$ polymerized acenaphthylene
 (II) by means of a carbanion chain. By the simultaneous presence of
 Ph_3Al , the 1st step in the polymerization was halted after 1,2-addition of I
 to II by formation of III. In the presence of Ph_3B , however, a 1,6-addition
 occurred, which formed IV. The acid hydrolysis of IV gave V, easily
 isomerized to 1-tritylacenaphthene (VI). The process leading to the
 formation of IV was explained by a π -complex formation between Ph_3B and
 II. Thermal decomposition of trimethylammonium tetraphenylborate gave Ph_3B , m.
 $151-2^\circ$ ($\text{Me}_2\text{CO-H}_2\text{O}$). In 1 compartment of a double Schlenk tube was
 dissolved 9.5 millimoles Ph_3B in 70 cc. absolute Et_2O by warming under N, the
 solution filtered into the other compartment, treated with 9.5 millimoles I
 in 95 cc. Et_2O , and cooled to -70° to give the at-complex I.BPh₃.
 II m. $92-2.5^\circ$ (70% EtOH). II (42 millimoles) in 20 cc. absolute Et_2O
 added slowly from 1 compartment of a double Schlenk tube to 43 millimoles
 Ph_3B in 360 cc. 0.09M $\text{Et}_2\text{O-I}$ contained in the other compartment, after 10
 min. the precipitate (IV) filtered off under N, washed with Et_2O under N,
 dissolved in 220 cc. distilled H_2O , the solution acidified to pH 1 with 2N HCl ,
 and extracted with 3:2 $\text{Et}_2\text{O-C}_6\text{H}_6$ gave 1.5 g. V, m. $184-5^\circ$ (decomposition)
 ($\text{CHCl}_3\text{-EtOH}$). A sample of V dissolved in boiling AcOH and cooled gave VI,
 m. $241-2^\circ$ (decomposition) [tetrahydrofuran (THF)- EtOH]. The mother
 liquors of V chromatographed on Al_2O_3 yielded addnl. V. Concentration of the
 Et_2O solution decanted from IV gave 14% (Ph_3C) $_2\text{O}_2$, m. $185-6^\circ$
 (dioxane); the Et_2O filtrate washed with aqueous NaOH to remove Ph_3B ,
 evaporated,
 the residue chromatographed on Al_2O_3 in CCl_4 and eluted with CCl_4 gave 30%
 II, m. $91-2^\circ$ (70% EtOH); further elution with CHCl_3 gave 14%
 Ph_3COH , m. $161-2^\circ$ (cyclohexane). To 6 g. $\text{Ph}_3\text{Al.Et}_2\text{O}$ in 10 cc. absolute
 Et_2O was added 16 millimoles I in 150 cc. Et_2O , the mixture treated with 16
 millimoles II in 10 cc. absolute Et_2O , shaken 45 hrs., heated 12 hrs. at
 50° , the solution decomposed with 200 cc. 2N NaOH (all operations under
 N), and the precipitate filtered off to give 35% (including addnl. material
 from
 filtrate) crude VI, m. 230° . Li-Hg (from 100 g. Hg and 0.2 g. Li)
 was treated with 3.5 g. Ph_3CCl (m. 113°) in 550 cc. absolute Et_2O , the
 mixture shaken overnight, and the solution transferred to a stock burette to
 give $\text{Ph}_3\text{CLi.Et}_2\text{O}$; its content was determined by hydrolysis of an aliquot and
 titration with HCl . Ph_3CLi (8 millimoles) in 500 cc. Et_2O added to 8
 millimoles 1-bromoacenaphthylene (m. $69-70^\circ$) in 20 cc. absolute Et_2O ,
 the solution concentrated to 50 cc., the precipitate filtered off, and washed
 with H_2O
 gave 98% VI, m. $241-2^\circ$ (THF- EtOH). A sample of VI (m.
 $241-2^\circ$) heated in vacuo while the bath temperature was gradually raised
 to 250° gave (at 0.2 mm.) II and (at 0.02 mm.) a small amount of VI
 and Ph_3CH . To 3 millimoles VI in 140 cc. boiling AcOH was added dropwise

during 25 min. 60 millimoles CrO_3 in 600 cc. AcOH , the solution boiled 1 hr., concentrated to 80 cc., and poured into 200 cc. H_2O to give Ph_3COH , m. $163-4^\circ$ (MeOH with C); the aqueous filtrate treated with Na_2SO_3 and extracted 48 hrs. with 300 cc. Et_2O gave 1,8-naphthalic acid anhydride, m. $271-2^\circ$ (PhMe). NOCl (26 millimoles) in 25 cc. THF added dropwise during 5 min. to 12 millimoles VI in 250 cc. THF , after 30 min. the precipitate filtered off, and washed with 50 cc. THF gave 56% x-nitroso-y-chloro-1-trityldihydroacenaphthene (VII), m. $181-2^\circ$ (decomposition) ($\text{CHCl}_3\text{-EtOH}$). VII (1 g.) in 250 cc. AcOH boiled 20 min., the solution evaporated in vacuo,

and

the residue digested with 10 cc. MeOH gave 61% 2-acetoxy-1-tritylacenaphthene (VIII), m. $239-40^\circ$ (THF-EtOH). $\text{Pb}(\text{OAc})_4$ (2 g.) in 50 cc. CHCl_3 and 1 g. VI stirred 15 hrs., filtered, the filtrate concentrated, the residue washed with H_2O , taken up in THF , the solution filtered,

the filtrate concentrated, the residual tar dissolved in Et_2O , and the solution concentrated to small volume gave 61% VIII, m. $240-40.5^\circ$ (EtOH). VII (2 g.) in 2 l. AcOH boiled 15 hrs., the AcOH removed, the residue stirred with 20 cc. MeOH , and crystallized from AcOH gave 70% 1-tritylacenaphthylene (IX), m. $225-5.5^\circ$. IX was also obtained by boiling VIII in AcOH . 3,8-Dimethylacenaphthenone (m. $113-14^\circ$) (20 g.) in 1 l. absolute Et_2O added slowly with stirring to 5 g. LiAlH_4 in 200 cc. absolute Et_2O , the mixture boiled 3 hrs., treated with 500 cc. 2N HCl , and the Et_2O phase evaporated gave almost quant. 3,8-dimethyl-1-acenaphthenol (X), m. $114-15^\circ$ (petr. ether). X (16 g.) in 160 cc. absolute pyridine treated during 10 min. at 0° with 8 g. AcCl in 20 cc. dry CHCl_3 with stirring, kept 8 hrs. at 20° , poured into 1 l. H_2O , extracted with Et_2O , the extract washed with 4N HCl and aqueous NaHCO_3 , and fractionated gave 87% Ac derivative (XI) of X,

b0.01

120-3°, m. $63-4^\circ$ (MeOH). XI (10 g.) in 20 cc. quinoline and 180 cc. $(\text{HOCH}_2)_2$ (XII) boiled gently 30 min., cooled, poured into 500 cc. 4N HCl , extracted with Et_2O , the Et_2O phase washed with aqueous NaHCO_3 , and evaporated

gave 80% 3,8-dimethylacenaphthylene (XIII), m. $56.5-7.5^\circ$ (sublimation in vacuo, then 70% EtOH). XIII (5-millimoles) and 5 millimoles 1,3-diphenylisobenzofuran (XIV) in 15 cc. absolute xylene heated 15 hrs. at 130° , diluted with 100 cc. petr. ether, the precipitate manually freed from yellow needles (unchanged XIV), dissolved in 10 cc. hot xylene, the solution filtered, and the filtrate diluted with 100 cc. EtOH gave 29% adduct, m. $195.5-6.0^\circ$; from the mother liquor was isolated 48% XIII and 58% XIV. To 110 millimoles Ph_3B suspended in 200 cc. absolute Et_2O was added 11 millimoles XIII followed during 30 min. by 11 millimoles I in 100 cc. Et_2O , after 12 hrs. the supernatant liquor decanted from a precipitate, the precipitate taken up in 100 cc. H_2O , the solution acidified with 2N HCl , the resulting precipitate dissolved in C_6H_6 , the solution washed with aqueous NaOH

(to

remove Ph_3B), and concentrated to 15 cc. to give 850 mg. Ph_3CH , m. $92-3^\circ$ (EtOH) (the mother liquor contained 300 mg. material, chiefly tar); the decanted Et_2O solution washed with aqueous NaOH , evaporated, the residue chromatographed on Al_2O_3 , and eluted with C_6H_6 gave 1.60 g. Ph_3CH , m. $88-92^\circ$ (from the mother liquor was isolated 20 mg.

p-benzhydryltetraphenylmethane (XV) and 14% XIII, m. $55-6.5^\circ$). An experiment with 2:1:1 $\text{Ph}_3\text{B-XIII-I}$ gave 91% Ph_3CH , 22% XIII, and 38% tar. Freshly distilled EtO_2CCOCl (0.31 mole) added at 0° to 0.31 mole AlCl_3 in 150 cc. PhNO_2 with stirring, the mixture treated dropwise during 1 hr. with 0.15 mole 1,8- $\text{ClO}_2\text{H}_6\text{Me}_2$ (m. $64-5^\circ$) at $0-5^\circ$, kept 12 hrs. at 15° , and decomposed with 1 l. 1:1 concentrated $\text{HCl-ice H}_2\text{O}$ with stirring gave 69% Et 4,5-dimethyl-1-naphthylglyoxylate (XVI), b0.01 $160-3^\circ$, m. $51-2^\circ$ (MeOH). XVI (75 g.) refluxed with 93 g. KOH and 116 g.

80% N₂H₄.H₂O in 580 cc. XII, diluted with 3 l. H₂O, filtered, and the filtrate acidified with concentrated HCl to pH 1 gave 86% 4,5-dimethyl-1-naphthaleneacetic acid (XVII), m. 184-5° (dilute EtOH with C). To 40 g. XVII in 500 cc. boiling CHCl₃ was added during 20 min. 51 g. freshly distilled SOCl₂ in an equal volume CHCl₃ with stirring, the mixture concentrated, the residual acid chloride taken up in 400 cc. PhNO₂, the solution added dropwise during 2 hrs. to 45 g. AlCl₃ in 300 cc. PhNO₂ (preheated to 70°) with stirring, stirred 36 hrs. at 20°, decomposed with 800 g. ice and 250 cc. concentrated HCl, the PhNO₂ phase steam distilled, the residue rubbed with MeOH, and sublimed at 160-5° (bath temperature)/0.01 mm. to give 70% 5,6-dimethylacenaphthenone (XVIII), m. 164-5° (EtOH with C). XVIII (25 g.) added to 10 g. LiAlH₄ in 1.2 l. absolute Et₂O with stirring, the mixture boiled 24 hrs., decomposed with 700 cc. 2N HCl, the precipitate present at the interphase filtered off, and combined with a slight amount product present in the Et₂O gave 80% 5,6-dimethyl-1-acenaphthanol (XIX), m. 192-3° (EtOH). To 20 g. XIX in 100 cc. absolute pyridine was added dropwise at 0° 16 g. AcCl in 20 cc. CHCl₃ with stirring, the mixture stirred 12 hrs. at 0°, decomposed with 600 cc. H₂O, and the product isolated with Et₂O to give 90% Ac derivative (XX) of XIX, m. 84-5° (EtOH). XX (10 g.) in 20 cc. quinoline and 180 cc. XII boiled gently 30 min., decomposed with HCl, the crude product isolated with Et₂O (as described for XIII), pulverized, extracted with petr. ether, the extract concentrated to 100 cc., chromatographed on Al₂O₃, and eluted with petr. ether gave 64% 5,6-dimethylacenaphthylene (XXI), m. 98-9° (petr. ether with C). XXI (5.26 millimoles) in 20 cc. EtOAc added to a prereduced suspension of 0.2 g. Pd-C in 15 cc. EtOAc and 5 cc. MeOH (after shaking 1 hr. 5.23 millimoles H absorbed) gave 5,6 dimethylacenaphthene, m. 167-9° (EtOH). XXI (5 millimoles) and 5 millimoles XIV in 15 cc. xylene heated 15 hrs. at 130° under N and diluted with 100 cc. petr. ether gave 84% adduct, m. 213.5-14.5° (iso-AmOH); from the mother liquor was isolated 10% XXI. To 23 millimoles Ph₃B suspended in 20 millimoles I in 170 cc. Et₂O was added gradually 20 millimoles XXI, the mixture shaken vigorously (the Ph₃B dissolved), after 1 hr. shaken and cooled to 0°, kept 12 hrs., the supernatant liquor decanted from the precipitate, the precipitate washed with absolute Et₂O, dissolved in 2 l. H₂O, the solution acidified, extracted with Et₂O, the extract washed with aqueous NaOH, and concentrated to 20 cc. to give 2.1 g. crude 1-trityl-5,6-dimethylacenaphthene (XXII); a sample dissolved in a little CHCl₃, the solution diluted with EtOH, and cooled to -50° gave XXII, m. 238-40° (CHCl₃-EtOH); the remaining crude XXII dissolved in boiling AcOH and the solution boiled 5 min. gave XXII, m. 256-8°, which was recrystd. 3 times from 95% BuOH to give XXII, m. 259-60° (decomposition), mixed m.p. (with material m. 238-40°) 238-43°; the infrared spectra of both preps. were practically identical. PBr₃ (7 g.) in 10 cc. absolute Et₂O added dropwise with stirring to 3 g. XIX in 150 cc. absolute Et₂O at 0°, kept 1.5 hrs. at 0°, diluted with sufficient absolute Et₂O to effect solution, the solution washed rapidly with dilute aqueous NaHCO₃, dried, added with stirring to 0.1N I-Et₂O until a permanent red color formed, and treated with H₂O gave XXII, m.p. and mixed m.p. 259-60° (95% BuOH). 5,6-Dichloroacenaphthene (XXIII) (m. 167-8°) (58 g.) in 1 l. AcOH (distilled over KMnO₄) treated portionwise at 65° with 210 g. Pb₃O₄, heated 1 hr. at 80-90°, the solution poured into 2 l. ice H₂O, the supernatant solution decanted from a gummy precipitate, the precipitate dissolved in 400 cc. hot EtOH, the

solution treated with C, and cooled gave 1-acetoxy derivative (XXIV) of XXIII, m.

104-5° (EtOH). XXIV (50 g.) boiled 1.5 hrs. with 30 g. KOH in 500 cc. MeOH and diluted with 500 cc. H₂O gave 80% 5,6-dichloro-1-acenaphthenol (XXV), m. 157-8° (C₆H₆ with C). XXV (30 g.) in 500 cc. C₆H₆ and a minute amount 4-MeC₆H₄SO₃H heated 30 min. under a H₂O separator (2 cc. H₂O was formed), the solution washed with aqueous NaOH, concentrated, the residue taken up

in petr. ether, the filtered solution chromatographed on Al₂O₃, and eluted with petr. ether gave 49% 5,6-dichloroacenaphthylene (XXVI), m. 161-1.5°. To 46 millimoles Ph₃B and 20 millimoles XXVI in 150 cc. absolute Et₂O was added portionwise 20 millimoles I in 200 cc. Et₂O with stirring and the complex worked up as above to give 21% 1-trityl derivative of XXVI, m. 240-1° (decomposition) (BuOH); the Et₂O solution yielded 8% XXVI, 39% Ph₃CH, 3% XV, and 5% tar. The following compds. were prepared for spectral comparison studies. Finely powdered Ph₃P.MeBr (65 millimoles) added to 60 millimoles BuLi in 100 cc. Et₂O in an N atmospheric, the mixture shaken

0.5 hr., the solution of Ph₃P:CH₂ (XXVII) treated dropwise with 50 millimoles OC.CMe₂.CH:CH.C₆H₄ (XXVIII) (b₁₅ 130.5-2.0°, n_{24D} 1.5705) in 30 cc.

absolute Et₂O (exothermic reaction), shaken 40 hrs. at room temperature, decanted

from precipitated Ph₃PO, the Et₂O phase and washings combined, treated with N NaOH, concentrated to 30 cc., filtered from more Ph₃PO, and the filtrate worked up gave 5.2 g. H₂C:C.CMe₂.CH:CH.C₆H₄ (XXIX), b_{0.3} 55.5-7.0°, n_{25D} 1.5757, and Ph₃PO (the total yield of Ph₃PO was 8.6 g.). XXIX (10.4 millimoles in 40 cc. EtOAc hydrogenated with 0.3 g. Pd-C (20.7 millimoles H absorbed in 4 hrs.) gave 85% MeCH.CMe₂.CH₂.CH₂.C₆H₄ (XXX), b₁₆ 113-14°. OC.CMe₂.CH₂.CH₂.C₆H₄ (XXXI) (b₁₅ 131-2°, n_{20D} 1.5424 (29 millimoles) in 50 cc. absolute Et₂O treated as above with 36 millimoles XXVII in 80 cc. Et₂O gave 4.2 g. H₂C:C.CMe₂.CH₂.CH₂.C₆H₄ (XXXII), b₁₅ 118.5-20.0°, n_{20D} 1.5570. XXXII (2.3 g.) in 60 cc. EtOAc hydrogenated with 0.3 g. Pd-C gave XXX, b₁₆ 114-15°, n_{19.5D} 1.5274, identical with XXX prepared above. To Ph₃P:CHMe (XXXIII) solution (prepared from 65 millimoles Ph₃P.EtBr and 61 millimoles BuLi in 100 cc. Et₂O) was added slowly 41 millimoles XXVIII in 50 cc. absolute Et₂O, shaken 1 week at room temperature, and worked up as usual to give 8.1 g. Ph₃PO and 5.1

g.

MeCH:C.CMe₂.CH:CH.C₆H₄ (XXXIV), b_{0.05} 62.5-3.0°, n_{18D} 1.5803. Hydrogenation of 10.4 millimoles XXXIV in 50 cc. EtOAc with 0.3 g. Pd-C (20.7 millimoles H absorbed in 4 hrs.) gave 83% EtCH.CMe₂.CH₂.CH₂.C₆H₄ (XXXV), b_{0.3} 56-7°, n_{20D} 1.5248. XXXI (40 millimoles) treated with 46 millimoles XXXIII in 120 cc. Et₂O and shaken 46 hrs. at 20° gave 6.5 g. MeCH:C.CMe₂.CH₂.CH₂.C₆H₄ (XXXVI), b_{0.4} 70-70.5°, n_{20D} 1.5568. Hydrogenation of 25 millimoles XXXVI in 50 cc. EtOAc with 0.5 g. Pd-C gave XXXV, b_{0.3} 56-7°, n_{20D} 1.5256, identical with XXXV prepared above. OC.CH:CH.CMe₂.C₆H₄ (XXXVII) (m. 69-70.5°) (50 millimoles) treated as above with 60 millimoles XXVII in 160 cc. Et₂O and heated 70 hrs. at 60° gave 43% Ph₃PO and 1.8 g. H₂C:C.CH:CH.CMe₂.C₆H₄, b_{0.1} 54-4.5°, n_{22D} 1.5807. XXXVII (50 millimoles) treated as above with 60 millimoles XXXIII in 160 cc. Et₂O and heated 50 hrs. at 60° gave 70% Ph₃PO and 4.7 g. MeCH:C.CH:CH.CMe₂.C₆H₄ (XXXVIII), b_{0.03} 69.5-70.0°, n_{22D} 1.5821. Hydrogenation (10 hrs.) of 6.4 millimoles XXXVIII in 60 cc. EtOAc with 0.5 g. Pd-C gave 1.2 g. EtCH.CH₂.CH₂.CMe₂.C₆H₄ (XXXIX), b₁₄ 125-6°, n_{20D} 1.5215. EtMgBr solution (from 13 g. EtBr and 2.5 g. Mg in 40 cc. absolute Et₂O) combined at 0° with 10 g. OC.CH₂.CH₂.CMe₂.C₆H₄ (b_{0.3} 79-81°) in 30 cc. absolute Et₂O, boiled 90 min., and decomposed with aqueous NH₄Cl gave 9.5 g. HOCeT.CH₂.CH₂.CMe₂.C₆H₄ (XL), b₁₄ 98-8.5°, m. 60-1°. XL

(9.5 g.) and a minute amount 4-MeC₆H₄SO₃H boiled 12 hrs. under a H₂O separator, washed with aqueous NaHCO₃, and fractionated gave 88% EtC:CH.CH₂.CMe₂.C₆H₄ (XLI), b₁₄ 124.5-5.0°, n_{20D} 1.5503. Hydrogenation (25 min.) of 16.6 millimoles XLI in 60 cc. EtOAc with 0.5 g. Pd-C gave 3 g. XXXIX, b₁₄ 125-6°, n_{20D} 1.5217.

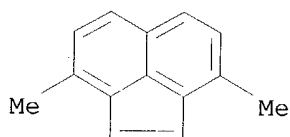
CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)

IT 7267-09-6, Acenaphthylene, 5,6-dichloro- **41002-80-6**, Acenaphthylene, 3,8-dimethyl- **41002-83-9**, Acenaphthylene, 5,6-dimethyl- (preparation and reactions of)

IT **41002-80-6**, Acenaphthylene, 3,8-dimethyl- **41002-83-9**, Acenaphthylene, 5,6-dimethyl- (preparation and reactions of)

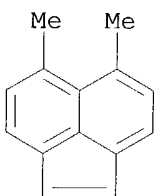
RN 41002-80-6 HCAPLUS

CN Acenaphthylene, 3,8-dimethyl- (6CI, 9CI) (CA INDEX NAME)



RN 41002-83-9 HCAPLUS

CN Acenaphthylene, 5,6-dimethyl- (6CI, 9CI) (CA INDEX NAME)



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